



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:28 AM UTC

PDB ID : 7CVT / pdb_00007cvt
Title : Crystal structure of the C85A/L194A/H234C mutant CLC-ec1 with Fab fragment
Authors : Park, K.; Mersch, K.; Robertson, J.; Lim, H.-H.
Deposited on : 2020-08-27
Resolution : 2.90 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

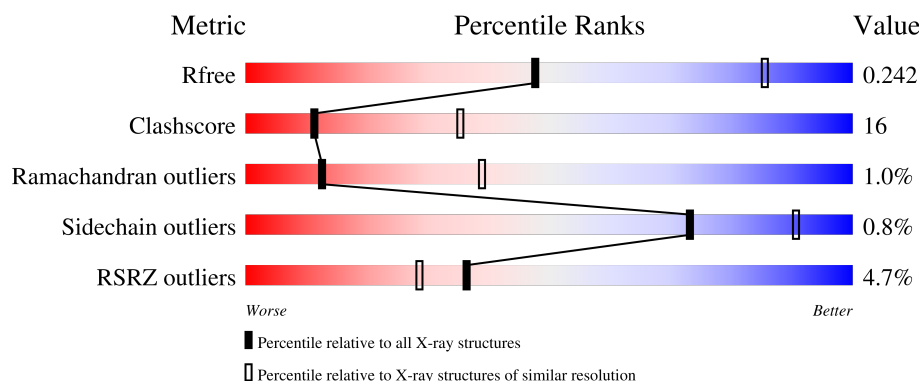
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	473	4% 67% 26% 6%
1	B	473	7% 59% 34% 6%
2	C	222	2% 79% 20%
2	E	222	4% 77% 23%
3	D	211	6% 63% 36%

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Mol	Chain	Length	Quality of chain
3	F	211	

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
4	CL	A	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13248 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3325	2184	558	563	20			
1	B	444	Total	C	N	O	S	0	0	0
			3325	2184	558	563	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	CYS	engineered mutation	UNP D7XDR7
A	194	ALA	LEU	engineered mutation	UNP D7XDR7
A	234	CYS	HIS	engineered mutation	UNP D7XDR7
B	85	ALA	CYS	engineered mutation	UNP D7XDR7
B	194	ALA	LEU	engineered mutation	UNP D7XDR7
B	234	CYS	HIS	engineered mutation	UNP D7XDR7

- Molecule 2 is a protein called antibody Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1681	1082	275	318	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called antibody Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest")

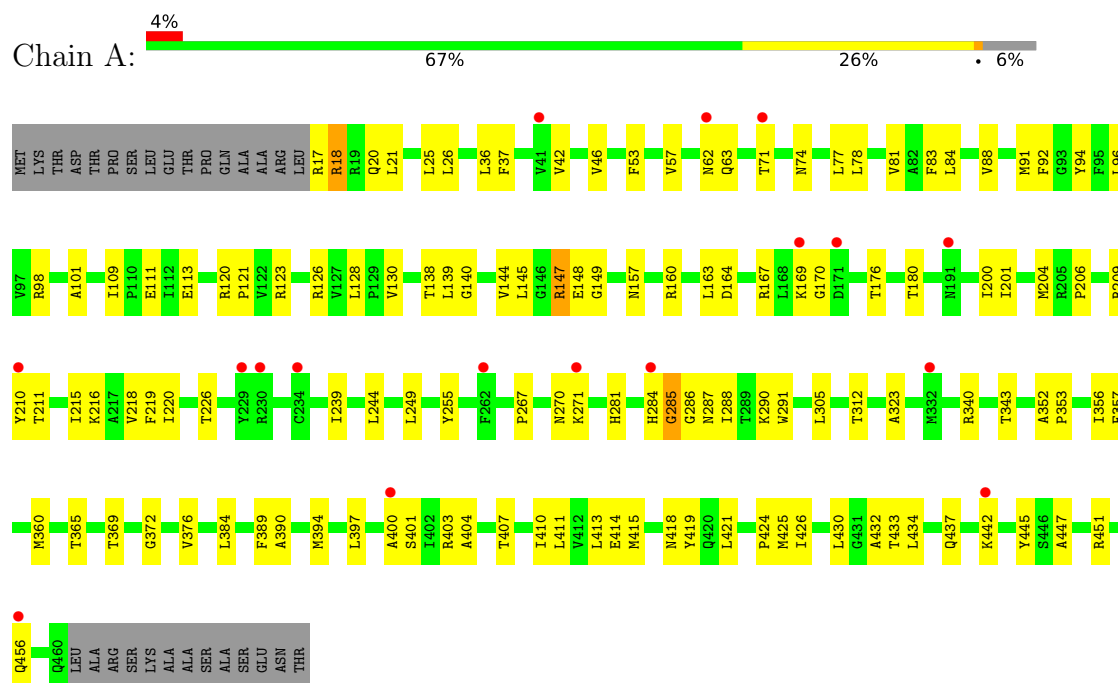
by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0
4	B	1	Total 1	Cl 1	0	0

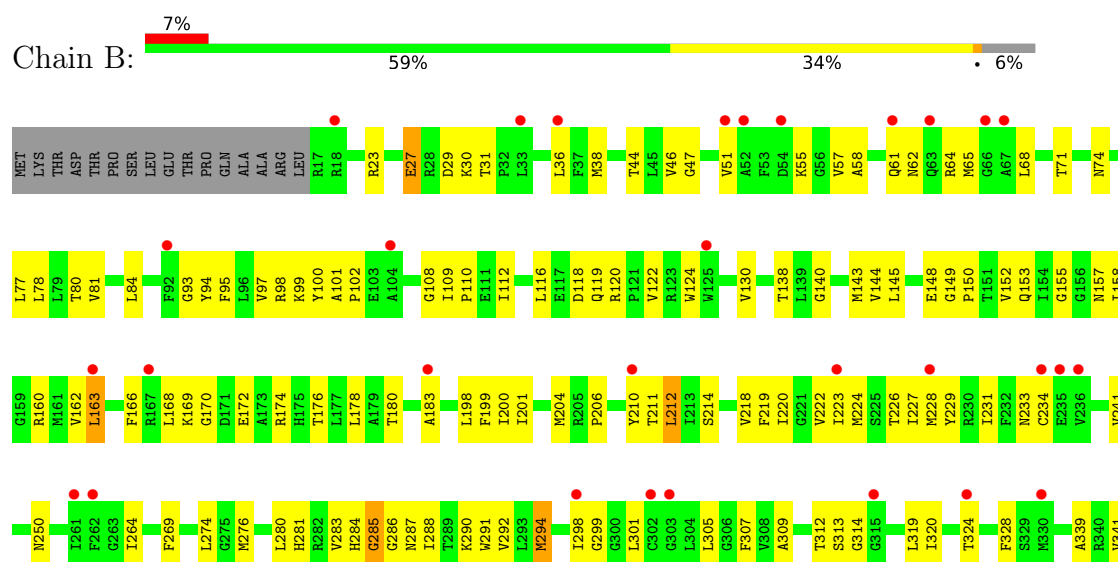
3 Residue-property plots

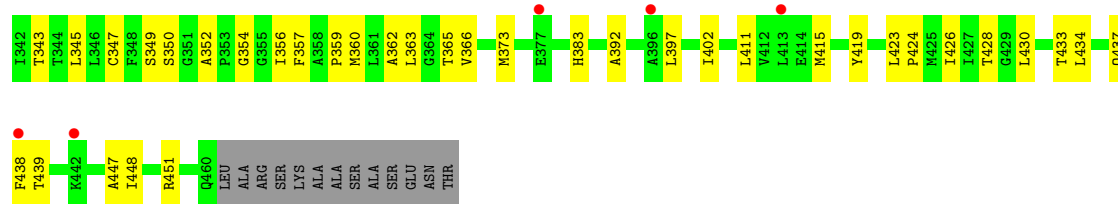
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

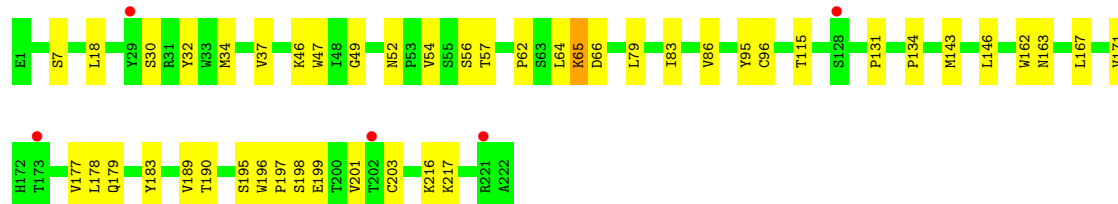
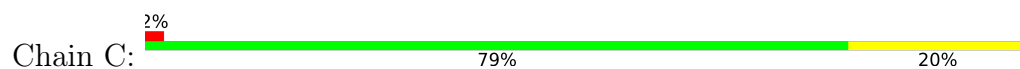


- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

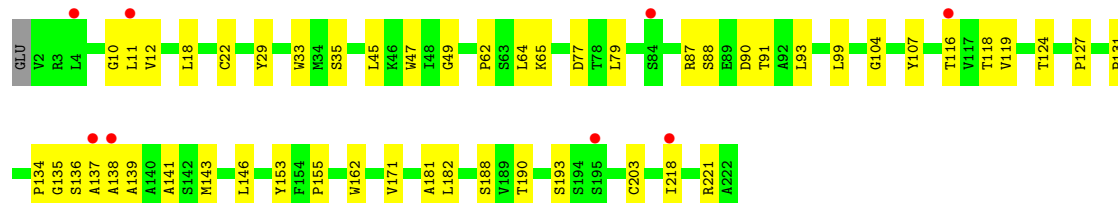
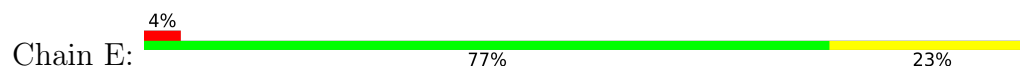




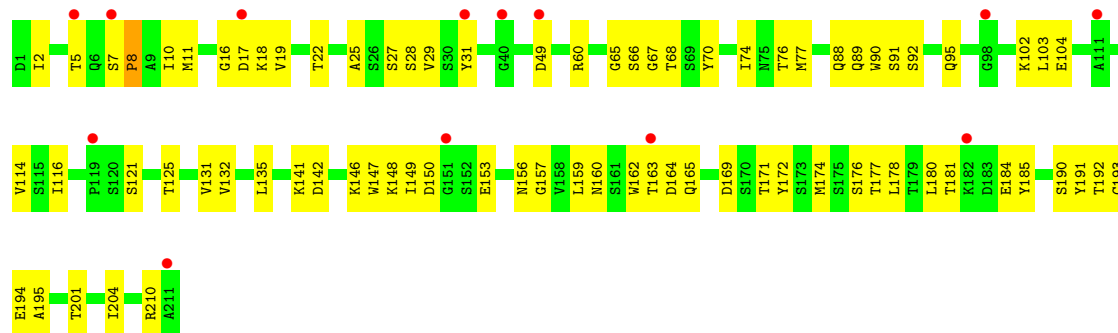
• Molecule 2: antibody Fab fragment heavy chain



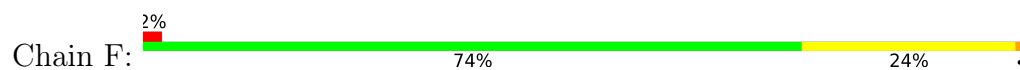
• Molecule 2: antibody Fab fragment heavy chain

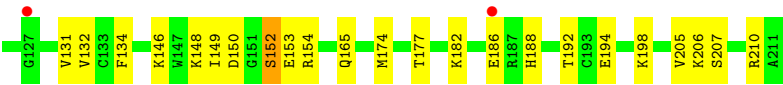


• Molecule 3: antibody Fab fragment light chain



• Molecule 3: antibody Fab fragment light chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.03Å 98.31Å 172.43Å 90.00° 131.99° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.90) 99.0 (50.00-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.201 , 0.241 0.202 , 0.242	Depositor DCC
R_{free} test set	3295 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	96.6	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 100.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13248	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: CL

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	0.22	0/3396	0.51	0/4609
1	B	0.27	0/3396	0.58	2/4609 (0.0%)
2	C	0.18	0/1730	0.44	0/2367
2	E	0.17	0/1721	0.39	0/2355
3	D	0.21	0/1660	0.49	0/2257
3	F	0.37	1/1660 (0.1%)	0.49	0/2257
All	All	0.25	1/13563 (0.0%)	0.50	2/18454 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	46	TRP	CA-C	-12.59	1.44	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	GLY	CA-C-N	5.36	124.62	120.33
1	B	108	GLY	C-N-CA	5.36	124.62	120.33

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	3325	0	3476	113	0
1	B	3325	0	3476	167	0
2	C	1681	0	1663	28	0
2	E	1672	0	1654	35	0
3	D	1621	0	1546	69	0
3	F	1621	0	1546	49	0
4	A	2	0	0	1	0
4	B	1	0	0	1	0
All	All	13248	0	13361	430	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 16.

All (430) 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)
3:D:141:LYS:NZ	3:D:172:TYR:CD2	1.77	1.49
3:D:141:LYS:NZ	3:D:172:TYR:CE2	1.85	1.44
1:B:138:THR:CG2	1:B:143:MET:HE2	1.87	1.04
1:B:138:THR:HG23	1:B:143:MET:HE2	1.40	1.01
1:B:71:THR:HG23	1:B:77:LEU:HG	1.45	0.96
3:D:77:MET:HE1	3:D:103:LEU:HD23	1.49	0.95
1:B:319:LEU:HD12	1:B:320:ILE:N	1.83	0.94
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.50	0.92
1:A:456:GLN:O	1:A:456:GLN:NE2	2.03	0.91
1:A:219:PHE:HD1	1:B:430:LEU:HD13	1.36	0.91
3:F:7:SER:HB2	3:F:22:THR:H	1.36	0.89
1:A:372:GLY:HA2	1:A:389:PHE:HD2	1.39	0.88
3:D:77:MET:HE1	3:D:103:LEU:CD2	2.03	0.87
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.41	0.86
1:B:109:ILE:O	1:B:112:ILE:HG22	1.75	0.86
1:B:110:PRO:HG2	1:B:448:ILE:HD11	1.57	0.85
1:B:298:ILE:HD12	1:B:299:GLY:N	1.93	0.84
3:D:169:ASP:HB3	3:D:171:THR:HG23	1.60	0.83
1:A:219:PHE:HD1	1:B:430:LEU:CD1	1.93	0.82
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.80	0.81
2:E:11:LEU:HD23	2:E:11:LEU:H	1.45	0.79
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.17	0.79
3:F:186:GLU:HG2	3:F:210:ARG:NH1	1.98	0.79
3:D:141:LYS:CE	3:D:172:TYR:CE2	2.65	0.78
1:B:64:ARG:NH2	1:B:140:GLY:O	2.12	0.77
1:B:264:ILE:HG22	1:B:439:THR:HG21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:HB2	1:A:77:LEU:HB3	1.68	0.76
1:B:110:PRO:CG	1:B:448:ILE:HD11	2.16	0.75
1:B:169:LYS:HG2	1:B:170:GLY:H	1.51	0.75
1:B:360:MET:HE1	1:B:402:ILE:HD13	1.69	0.74
3:F:182:LYS:O	3:F:186:GLU:HG3	1.87	0.74
1:B:62:ASN:HA	1:B:65:MET:HB2	1.69	0.74
2:C:171:VAL:HG22	2:C:189:VAL:HG12	1.68	0.74
3:D:160:ASN:OD1	3:D:176:SER:HB2	1.88	0.74
1:A:169:LYS:HG2	1:A:170:GLY:H	1.53	0.74
1:B:138:THR:HG22	1:B:143:MET:HE2	1.70	0.74
1:B:210:TYR:HE1	1:B:212:LEU:HD12	1.52	0.73
3:D:132:VAL:HG22	3:D:177:THR:HG23	1.71	0.73
1:B:110:PRO:CB	1:B:448:ILE:HD11	2.19	0.72
1:A:284:HIS:HA	1:A:290:LYS:HG2	1.72	0.71
3:F:7:SER:OG	3:F:8:PRO:HD3	1.91	0.71
1:A:369:THR:HG22	1:A:390:ALA:HB2	1.73	0.70
3:D:10:ILE:HD12	3:D:102:LYS:HB3	1.72	0.70
1:B:319:LEU:HD12	1:B:319:LEU:C	2.16	0.70
1:A:113:GLU:HG3	1:A:204:MET:HG2	1.72	0.70
1:A:92:PHE:O	1:A:96:LEU:HD12	1.92	0.70
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.73	0.70
3:D:141:LYS:HE3	3:D:172:TYR:CZ	2.27	0.70
3:D:95:GLN:OE1	3:D:95:GLN:N	2.24	0.69
1:A:88:VAL:HA	1:A:91:MET:HE2	1.72	0.69
1:B:57:VAL:O	1:B:61:GLN:HG3	1.93	0.69
1:A:219:PHE:CD1	1:B:430:LEU:CD1	2.76	0.69
3:D:163:THR:HG22	3:D:164:ASP:O	1.92	0.69
1:B:138:THR:CG2	1:B:143:MET:CE	2.68	0.68
1:B:138:THR:HG23	1:B:143:MET:CE	2.21	0.68
2:E:135:GLY:O	2:E:137:ALA:N	2.26	0.68
1:A:164:ASP:O	1:A:167:ARG:HD2	1.94	0.68
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.58	0.68
1:B:98:ARG:HH21	1:B:102:PRO:HB3	1.57	0.67
2:E:91:THR:HG22	2:E:119:VAL:H	1.60	0.67
1:B:160:ARG:HA	1:B:163:LEU:HB3	1.75	0.67
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.77	0.67
1:B:345:LEU:O	1:B:349:SER:OG	2.13	0.67
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.76	0.66
1:B:284:HIS:O	1:B:286:GLY:N	2.27	0.66
1:A:372:GLY:HA2	1:A:389:PHE:CD2	2.29	0.66
1:B:99:LYS:HG2	1:B:100:TYR:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ILE:HD12	1:A:288:ILE:H	1.60	0.65
2:E:93:LEU:HD13	2:E:116:THR:HG22	1.79	0.65
2:C:52:ASN:ND2	2:C:57:THR:H	1.93	0.65
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.78	0.64
2:C:131:PRO:HD3	2:C:216:LYS:HE2	1.79	0.64
3:D:29:VAL:O	3:D:70:TYR:OH	2.15	0.64
1:B:163:LEU:O	1:B:163:LEU:HD12	1.98	0.64
1:B:360:MET:HB3	1:B:397:LEU:HD22	1.80	0.64
1:A:42:VAL:O	1:A:46:VAL:HG23	1.98	0.64
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.79	0.64
1:A:365:THR:O	1:A:369:THR:HG23	1.98	0.63
1:B:61:GLN:HA	1:B:64:ARG:NH2	2.13	0.63
1:A:430:LEU:HA	1:A:433:THR:HG22	1.79	0.63
3:D:89:GLN:NE2	3:D:92:SER:H	1.96	0.63
1:A:244:LEU:H	1:A:418:ASN:ND2	1.96	0.63
1:B:162:VAL:HG23	1:B:166:PHE:CE2	2.33	0.63
1:B:284:HIS:C	1:B:286:GLY:H	2.07	0.63
3:F:149:ILE:O	3:F:152:SER:N	2.30	0.63
3:D:2:ILE:HD13	3:D:29:VAL:CG1	2.28	0.63
3:F:2:ILE:H	3:F:2:ILE:HD12	1.63	0.62
1:B:98:ARG:HE	1:B:98:ARG:HA	1.65	0.62
1:B:27:GLU:OE1	1:B:30:LYS:HD2	2.00	0.62
2:E:131:PRO:HB2	2:E:218:ILE:HG23	1.79	0.62
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.15	0.62
3:F:105:ILE:H	3:F:165:GLN:HE22	1.47	0.62
1:B:64:ARG:O	1:B:68:LEU:HD12	2.00	0.62
1:A:270:ASN:OD1	1:A:401:SER:OG	2.17	0.62
1:A:147:ARG:HG2	1:A:147:ARG:NH1	2.15	0.61
1:B:223:ILE:HG13	1:B:224:MET:N	2.14	0.61
2:E:91:THR:CG2	2:E:119:VAL:H	2.12	0.61
3:F:149:ILE:HD11	3:F:154:ARG:HB2	1.81	0.61
1:A:413:LEU:HD11	1:A:419:TYR:HD1	1.65	0.61
3:F:194:GLU:HA	3:F:205:VAL:HG12	1.81	0.61
1:A:71:THR:HG23	1:A:77:LEU:HG	1.81	0.61
1:B:148:GLU:HG2	1:B:149:GLY:N	2.15	0.61
3:D:153:GLU:OE2	3:D:153:GLU:N	2.33	0.61
1:B:430:LEU:HA	1:B:433:THR:HG22	1.83	0.60
1:A:83:PHE:HD1	1:A:84:LEU:HD12	1.67	0.60
1:A:403:ARG:NH2	1:B:29:ASP:O	2.35	0.60
1:B:61:GLN:HA	1:B:64:ARG:HH22	1.66	0.60
3:D:2:ILE:HD11	3:D:25:ALA:HB1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:160:ASN:OD1	3:D:176:SER:CB	2.49	0.60
1:B:58:ALA:O	1:B:61:GLN:HB2	2.01	0.60
3:F:148:LYS:HB2	3:F:192:THR:HB	1.83	0.60
1:B:309:ALA:O	1:B:312:THR:OG1	2.18	0.60
1:B:116:LEU:HG	1:B:178:LEU:HD23	1.84	0.60
3:D:104:GLU:OE2	3:D:165:GLN:NE2	2.35	0.59
3:D:181:THR:HG23	3:D:184:GLU:HG2	1.84	0.59
2:C:143:MET:HE3	2:C:190:THR:HG22	1.83	0.59
1:B:23:ARG:HG3	1:B:23:ARG:O	2.03	0.59
1:B:27:GLU:OE1	1:B:27:GLU:HA	2.03	0.59
1:B:356:ILE:N	4:B:501:CL:CL	2.70	0.59
1:B:424:PRO:O	1:B:428:THR:HG22	2.02	0.59
2:C:52:ASN:HD21	2:C:56:SER:N	2.01	0.59
2:C:79:LEU:HD23	2:C:96:CYS:SG	2.42	0.59
1:A:255:TYR:CE2	1:A:424:PRO:HB2	2.38	0.59
1:A:219:PHE:CD1	1:B:430:LEU:HD13	2.28	0.58
3:F:114:VAL:HG13	3:F:206:LYS:HG3	1.86	0.58
2:E:45:LEU:HD21	3:F:43:PRO:HG2	1.84	0.58
1:B:392:ALA:HB1	1:B:428:THR:HG21	1.84	0.58
1:B:320:ILE:HG23	1:B:365:THR:HG21	1.86	0.58
1:B:328:PHE:O	1:B:373:MET:HE1	2.03	0.58
3:D:141:LYS:NZ	3:D:172:TYR:CZ	2.65	0.58
3:D:2:ILE:CD1	3:D:29:VAL:HG13	2.33	0.58
1:B:241:VAL:HG13	1:B:324:THR:HG21	1.85	0.58
3:F:150:ASP:OD2	3:F:188:HIS:HD2	1.87	0.58
1:B:74:ASN:HB2	1:B:77:LEU:HD23	1.86	0.57
3:D:141:LYS:CE	3:D:172:TYR:CZ	2.87	0.57
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.11	0.57
3:F:149:ILE:CD1	3:F:154:ARG:HB2	2.34	0.57
3:D:141:LYS:HG2	3:D:172:TYR:CD1	2.40	0.57
1:A:219:PHE:CZ	1:B:426:ILE:HG23	2.39	0.57
1:A:180:THR:HG22	1:A:218:VAL:HG22	1.87	0.57
1:B:148:GLU:HG3	1:B:357:PHE:HB3	1.87	0.57
1:B:109:ILE:HD12	1:B:199:PHE:HE2	1.70	0.57
2:C:37:VAL:HG13	2:C:95:TYR:HB2	1.86	0.57
1:B:274:LEU:HD21	1:B:448:ILE:HG22	1.86	0.56
1:B:77:LEU:O	1:B:81:VAL:HG23	2.05	0.56
1:B:276:MET:HG3	1:B:280:LEU:HD13	1.88	0.56
1:A:21:LEU:HG	1:A:25:LEU:HD11	1.88	0.56
3:F:114:VAL:HA	3:F:134:PHE:O	2.05	0.56
3:D:2:ILE:HD13	3:D:29:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:HG22	1:A:78:LEU:HA	1.88	0.56
1:A:201:ILE:HD11	1:A:215:ILE:HG12	1.88	0.56
3:D:195:ALA:HB3	3:D:204:ILE:HG23	1.88	0.56
3:F:122:GLU:OE2	3:F:122:GLU:N	2.36	0.56
2:E:124:THR:HG22	2:E:155:PRO:HD3	1.86	0.56
1:A:120:ARG:NH1	1:A:121:PRO:HD2	2.21	0.55
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.88	0.55
1:A:356:ILE:O	1:A:360:MET:HG3	2.07	0.55
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.40	0.55
1:B:109:ILE:HD13	1:B:152:VAL:HG11	1.88	0.55
3:D:17:ASP:OD1	3:D:18:LYS:N	2.40	0.55
3:D:163:THR:HG22	3:D:164:ASP:N	2.21	0.55
1:A:201:ILE:HG21	1:B:201:ILE:HD13	1.86	0.55
2:C:178:LEU:HB2	2:C:183:TYR:CE1	2.42	0.55
1:A:219:PHE:CD1	1:B:430:LEU:HD12	2.42	0.55
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.88	0.55
1:B:176:THR:O	1:B:180:THR:HG23	2.07	0.55
3:D:27:SER:OG	3:D:28:SER:N	2.40	0.55
3:D:77:MET:CE	3:D:103:LEU:CD2	2.83	0.54
1:A:403:ARG:NH2	1:A:437:GLN:HB2	2.23	0.54
1:A:426:ILE:HG23	1:B:219:PHE:CE1	2.42	0.54
1:B:144:VAL:O	1:B:144:VAL:HG23	2.07	0.54
1:B:281:HIS:O	1:B:285:GLY:N	2.40	0.54
1:B:319:LEU:HD12	1:B:320:ILE:CA	2.37	0.54
3:F:109:ASP:OD1	3:F:198:LYS:HE2	2.06	0.54
1:B:222:VAL:O	1:B:226:THR:HG22	2.08	0.54
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.89	0.54
2:E:143:MET:HE3	2:E:190:THR:HG22	1.88	0.54
1:A:176:THR:O	1:A:180:THR:HG23	2.06	0.53
1:B:47:GLY:O	1:B:51:VAL:HG23	2.09	0.53
2:C:163:ASN:HB2	2:C:167:LEU:HD12	1.91	0.53
3:F:7:SER:CB	3:F:22:THR:H	2.15	0.53
3:F:186:GLU:HG2	3:F:210:ARG:CZ	2.39	0.53
1:B:158:ILE:O	1:B:162:VAL:HG12	2.09	0.53
3:D:116:ILE:HD11	3:D:147:TRP:CZ3	2.43	0.53
1:A:148:GLU:HG3	1:A:357:PHE:HB3	1.91	0.53
1:A:244:LEU:H	1:A:418:ASN:HD21	1.56	0.53
1:A:287:ASN:HB3	1:A:290:LYS:HE3	1.90	0.53
3:D:149:ILE:HD13	3:D:191:TYR:HE2	1.72	0.53
3:F:7:SER:OG	3:F:8:PRO:CD	2.57	0.53
1:B:95:PHE:CE1	1:B:99:LYS:HD3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:TYR:CE1	1:B:212:LEU:HD12	2.38	0.53
1:B:219:PHE:O	1:B:223:ILE:HG23	2.08	0.53
3:F:152:SER:OG	3:F:153:GLU:N	2.41	0.53
1:A:249:LEU:HD11	1:B:234:CYS:SG	2.49	0.52
1:B:313:SER:OG	1:B:314:GLY:N	2.42	0.52
2:C:162:TRP:CG	2:C:189:VAL:HG11	2.44	0.52
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.91	0.52
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.44	0.52
3:D:88:GLN:HG2	3:D:89:GLN:N	2.23	0.52
1:A:305:LEU:HB3	1:A:312:THR:OG1	2.09	0.52
1:B:153:GLN:O	1:B:157:ASN:ND2	2.36	0.52
1:B:210:TYR:HE1	1:B:212:LEU:CD1	2.20	0.52
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.45	0.52
3:D:150:ASP:HA	3:D:190:SER:HB3	1.92	0.52
3:F:186:GLU:HG2	3:F:210:ARG:NH2	2.25	0.52
1:B:319:LEU:C	1:B:319:LEU:CD1	2.83	0.52
3:D:2:ILE:HG21	3:D:89:GLN:NE2	2.25	0.52
3:D:131:VAL:HG13	3:D:178:LEU:HB3	1.93	0.51
1:B:198:LEU:HD13	1:B:201:ILE:HD11	1.93	0.51
1:A:365:THR:HG22	1:A:394:MET:HB2	1.92	0.51
1:B:110:PRO:HB2	1:B:448:ILE:HD11	1.93	0.51
2:C:52:ASN:OD1	2:C:54:VAL:N	2.44	0.51
3:D:180:LEU:HB3	3:D:184:GLU:HG3	1.91	0.51
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.93	0.51
1:B:298:ILE:HD12	1:B:299:GLY:H	1.70	0.51
1:B:122:VAL:HG13	1:B:160:ARG:HG2	1.92	0.51
1:A:113:GLU:CG	1:A:204:MET:HG2	2.39	0.51
1:A:219:PHE:CE1	1:B:426:ILE:HG23	2.45	0.51
1:B:284:HIS:HB2	1:B:290:LYS:HG3	1.92	0.51
1:A:414:GLU:HG2	1:B:419:TYR:HE1	1.77	0.50
1:B:360:MET:HA	1:B:363:LEU:HD12	1.94	0.50
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.80	0.50
3:D:95:GLN:H	3:D:95:GLN:CD	2.19	0.50
1:A:53:PHE:O	1:A:57:VAL:HG12	2.12	0.50
3:D:16:GLY:N	3:D:77:MET:O	2.34	0.50
3:D:29:VAL:CG1	3:D:89:GLN:HG3	2.42	0.50
3:F:186:GLU:HG2	3:F:210:ARG:HH22	1.77	0.50
1:B:180:THR:HG22	1:B:218:VAL:HG22	1.94	0.50
1:A:148:GLU:HG2	1:A:149:GLY:N	2.27	0.50
2:C:177:VAL:HG11	3:D:159:LEU:HD13	1.93	0.50
2:E:47:TRP:CE3	3:F:95:GLN:NE2	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ALA:HB2	1:B:200:ILE:HG12	1.94	0.49
2:E:134:PRO:HD3	2:E:146:LEU:HD23	1.94	0.49
1:B:124:TRP:CD1	1:B:160:ARG:HG3	2.47	0.49
1:B:437:GLN:HG2	1:B:438:PHE:CD2	2.47	0.49
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.94	0.49
1:B:27:GLU:OE1	1:B:30:LYS:CD	2.60	0.49
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.47	0.49
1:B:362:ALA:O	1:B:366:VAL:HG23	2.12	0.49
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.93	0.49
1:B:280:LEU:HD23	1:B:350:SER:HA	1.93	0.49
3:D:7:SER:CB	3:D:22:THR:HB	2.43	0.49
1:A:144:VAL:HG21	1:A:343:THR:HB	1.93	0.49
2:C:83:ILE:HG22	2:C:86:VAL:HG12	1.93	0.49
3:D:11:MET:HG3	3:D:103:LEU:HD12	1.94	0.49
1:B:227:ILE:O	1:B:231:ILE:HG13	2.12	0.49
1:B:51:VAL:O	1:B:55:LYS:HG3	2.13	0.48
1:B:200:ILE:HA	1:B:204:MET:HB2	1.94	0.48
1:B:93:GLY:O	1:B:97:VAL:HG22	2.12	0.48
3:F:94:PRO:HB2	3:F:95:GLN:NE2	2.27	0.48
3:D:89:GLN:HG2	3:D:91:SER:H	1.79	0.48
2:E:10:GLY:O	2:E:118:THR:N	2.36	0.48
1:A:111:GLU:OE1	1:A:120:ARG:NH2	2.45	0.47
1:A:226:THR:HG21	1:B:423:LEU:HD11	1.95	0.47
1:B:99:LYS:HG2	1:B:100:TYR:CD1	2.49	0.47
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.49	0.47
3:F:2:ILE:HD11	3:F:92:SER:HB2	1.96	0.47
1:A:281:HIS:O	1:A:285:GLY:N	2.44	0.47
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.96	0.47
1:B:112:ILE:HD11	1:B:178:LEU:HD11	1.96	0.47
3:D:60:ARG:HB2	3:D:74:ILE:HG23	1.95	0.47
2:E:11:LEU:HA	2:E:118:THR:O	2.14	0.47
1:A:219:PHE:CE1	1:B:430:LEU:HB2	2.49	0.47
1:A:267:PRO:O	1:A:271:LYS:HD3	2.14	0.47
1:B:109:ILE:CD1	1:B:152:VAL:HG11	2.44	0.47
2:C:195:SER:O	2:C:199:GLU:N	2.41	0.47
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.95	0.47
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.96	0.47
1:A:287:ASN:HB3	1:A:290:LYS:CE	2.44	0.47
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.96	0.47
1:B:298:ILE:HD12	1:B:298:ILE:C	2.37	0.47
2:C:179:GLN:OE1	3:D:159:LEU:HD11	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:VAL:HG22	3:D:74:ILE:HB	1.95	0.47
1:A:287:ASN:OD1	1:A:287:ASN:C	2.57	0.47
1:B:57:VAL:HG12	1:B:61:GLN:HE21	1.80	0.47
1:A:92:PHE:CE1	1:A:96:LEU:HD11	2.50	0.47
1:A:128:LEU:HD21	1:A:157:ASN:HB2	1.96	0.47
3:D:147:TRP:O	3:D:153:GLU:HA	2.15	0.47
1:B:284:HIS:C	1:B:286:GLY:N	2.73	0.46
2:C:65:LYS:HG3	2:C:66:ASP:OD2	2.15	0.46
1:B:172:GLU:O	1:B:176:THR:HG23	2.15	0.46
1:A:404:ALA:O	1:A:407:THR:HG22	2.15	0.46
1:A:109:ILE:HG23	1:A:204:MET:SD	2.56	0.46
1:B:241:VAL:CG1	1:B:324:THR:HG21	2.45	0.46
3:F:94:PRO:HB2	3:F:95:GLN:HE22	1.81	0.46
1:A:403:ARG:NH2	1:B:29:ASP:OD2	2.46	0.46
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.97	0.46
1:B:356:ILE:O	1:B:360:MET:HG3	2.16	0.46
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.34	0.46
2:E:87:ARG:NH1	2:E:90:ASP:OD1	2.49	0.46
2:E:141:ALA:O	2:E:193:SER:OG	2.25	0.46
1:A:36:LEU:HB2	1:A:220:ILE:HD12	1.97	0.46
1:A:36:LEU:HD21	1:B:438:PHE:HZ	1.80	0.45
1:B:274:LEU:CD2	1:B:448:ILE:HG22	2.46	0.45
1:B:411:LEU:O	1:B:415:MET:HG3	2.16	0.45
3:D:121:SER:O	3:D:125:THR:HG23	2.15	0.45
2:E:35:SER:HB2	2:E:99:LEU:HD11	1.98	0.45
1:B:229:TYR:O	1:B:233:ASN:HB2	2.16	0.45
2:E:11:LEU:HD13	2:E:124:THR:HG23	1.98	0.45
1:B:339:ALA:O	1:B:343:THR:HG23	2.17	0.45
1:A:249:LEU:HD12	1:A:249:LEU:H	1.81	0.45
3:F:12:SER:HB3	3:F:106:LEU:HD21	1.98	0.45
1:B:288:ILE:O	1:B:292:VAL:HG13	2.16	0.45
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.99	0.45
3:F:149:ILE:HD12	3:F:149:ILE:H	1.82	0.45
1:B:71:THR:HG22	1:B:78:LEU:HD12	1.99	0.45
3:D:165:GLN:HE21	3:D:165:GLN:HB2	1.63	0.45
3:D:185:TYR:CZ	3:D:210:ARG:HD3	2.52	0.45
3:F:38:LYS:HG2	3:F:83:ALA:HB2	1.99	0.45
1:A:160:ARG:HD3	1:A:163:LEU:HD23	1.98	0.45
1:B:31:THR:HB	1:B:36:LEU:HD21	1.99	0.45
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.52	0.45
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.99	0.45
2:E:181:ALA:O	2:E:182:LEU:HD23	2.17	0.45
3:F:75:ASN:O	3:F:76:THR:OG1	2.33	0.45
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.51	0.44
1:B:280:LEU:O	1:B:283:VAL:HG12	2.17	0.44
2:E:171:VAL:HA	2:E:188:SER:O	2.18	0.44
1:A:414:GLU:HG2	1:B:419:TYR:CE1	2.51	0.44
1:B:71:THR:HG21	1:B:81:VAL:HG21	1.99	0.44
1:A:36:LEU:HD21	1:B:438:PHE:CZ	2.53	0.44
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.53	0.44
1:A:411:LEU:HG	1:A:415:MET:HE2	2.00	0.44
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.98	0.44
3:D:114:VAL:HG22	3:D:135:LEU:HD13	1.98	0.44
3:D:135:LEU:HD11	3:D:195:ALA:HB2	1.99	0.44
1:A:271:LYS:HD2	1:A:271:LYS:N	2.33	0.44
1:B:44:THR:HG23	1:B:228:MET:HE3	2.00	0.44
3:F:95:GLN:N	3:F:95:GLN:CD	2.76	0.44
1:A:26:LEU:HD12	1:A:26:LEU:HA	1.85	0.44
1:A:74:ASN:OD1	1:A:74:ASN:N	2.50	0.44
2:C:146:LEU:CD1	2:C:201:VAL:HG11	2.48	0.44
1:B:46:VAL:HG22	1:B:155:GLY:HA2	1.98	0.44
2:E:10:GLY:N	2:E:116:THR:O	2.51	0.44
1:B:150:PRO:HD3	1:B:354:GLY:HA2	2.00	0.44
1:A:284:HIS:C	1:A:286:GLY:H	2.26	0.44
1:B:148:GLU:HG3	1:B:357:PHE:CB	2.47	0.44
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.86	0.44
1:A:123:ARG:NH2	1:A:126:ARG:HH21	2.16	0.43
1:A:139:LEU:CD2	1:A:145:LEU:HB2	2.48	0.43
1:A:430:LEU:HD21	1:B:223:ILE:HD13	2.01	0.43
1:A:447:ALA:O	1:A:451:ARG:HG3	2.18	0.43
1:B:71:THR:HG21	1:B:81:VAL:CG2	2.49	0.43
3:D:66:SER:O	3:D:68:THR:N	2.51	0.43
2:E:137:ALA:O	2:E:139:ALA:N	2.47	0.43
1:A:219:PHE:CD1	1:B:430:LEU:HB2	2.54	0.43
1:B:124:TRP:HD1	1:B:160:ARG:HG3	1.83	0.43
2:C:217:LYS:CD	2:C:217:LYS:H	2.31	0.43
3:D:7:SER:HB2	3:D:22:THR:HB	2.00	0.43
1:A:57:VAL:HG23	1:A:140:GLY:HA2	2.00	0.43
1:B:77:LEU:O	1:B:80:THR:HB	2.17	0.43
2:E:11:LEU:HD23	2:E:11:LEU:N	2.25	0.43
1:A:287:ASN:OD1	1:A:288:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:HB3	3:D:8:PRO:HD3	2.00	0.43
1:A:36:LEU:HD12	1:A:37:PHE:N	2.33	0.43
1:B:301:LEU:O	1:B:305:LEU:HD12	2.19	0.43
1:B:447:ALA:O	1:B:451:ARG:HG3	2.19	0.43
3:D:104:GLU:HB2	3:D:165:GLN:NE2	2.33	0.43
3:D:116:ILE:HD12	3:D:193:CYS:HB2	2.00	0.43
1:A:410:ILE:O	1:A:414:GLU:HG3	2.18	0.43
3:D:31:TYR:HB3	3:D:49:ASP:HA	2.00	0.43
1:B:294:MET:HE3	1:B:294:MET:HB2	1.78	0.42
1:A:200:ILE:HG22	1:A:201:ILE:HD12	2.01	0.42
1:B:163:LEU:HD22	1:B:174:ARG:HA	2.01	0.42
3:F:192:THR:HA	3:F:207:SER:HB3	2.01	0.42
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.55	0.42
1:A:18:ARG:H	1:A:18:ARG:HE	1.67	0.42
1:B:23:ARG:O	1:B:27:GLU:HB2	2.19	0.42
2:E:11:LEU:HD22	2:E:124:THR:CG2	2.49	0.42
1:A:209:ARG:HG3	1:A:210:TYR:O	2.20	0.42
1:B:145:LEU:HD11	1:B:347:CYS:HB3	2.00	0.42
3:D:89:GLN:HG2	3:D:90:TRP:N	2.34	0.42
1:A:77:LEU:O	1:A:81:VAL:HG23	2.20	0.42
1:B:94:TYR:HB3	1:B:292:VAL:HG12	2.01	0.42
1:B:112:ILE:CD1	1:B:178:LEU:HD11	2.50	0.42
1:B:176:THR:HG22	1:B:214:SER:H	1.85	0.42
3:F:186:GLU:HA	3:F:210:ARG:NH1	2.34	0.42
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.89	0.42
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.55	0.42
1:A:71:THR:CG2	1:A:78:LEU:HA	2.49	0.42
2:C:18:LEU:HD11	2:C:83:ILE:HD12	2.01	0.42
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.55	0.42
1:A:147:ARG:H	1:A:147:ARG:HG3	1.55	0.41
1:A:239:ILE:HD11	1:A:415:MET:HB3	2.00	0.41
2:E:11:LEU:H	2:E:11:LEU:CD2	2.24	0.41
1:A:71:THR:HG22	1:A:71:THR:O	2.20	0.41
1:A:340:ARG:HA	1:A:343:THR:OG1	2.20	0.41
1:B:287:ASN:O	1:B:290:LYS:HG2	2.20	0.41
2:C:46:LYS:HB3	2:C:46:LYS:HE3	1.78	0.41
3:F:105:ILE:H	3:F:165:GLN:NE2	2.16	0.41
3:F:174:MET:HB2	3:F:174:MET:HE3	1.79	0.41
1:A:62:ASN:OD1	1:A:63:GLN:N	2.52	0.41
2:C:7:SER:HA	2:C:115:THR:HG21	2.03	0.41
3:D:141:LYS:HZ1	3:D:172:TYR:HE2	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:SER:O	2:E:91:THR:OG1	2.33	0.41
3:F:20:THR:HG22	3:F:73:THR:OG1	2.20	0.41
1:A:323:ALA:HB1	1:A:369:THR:HG21	2.02	0.41
1:B:112:ILE:HD12	1:B:112:ILE:HA	1.90	0.41
1:B:120:ARG:HE	1:B:120:ARG:HB3	1.57	0.41
3:D:162:TRP:CE2	3:D:174:MET:HG3	2.56	0.41
3:F:194:GLU:HG2	3:F:205:VAL:HG12	2.03	0.41
1:A:360:MET:HG3	1:A:360:MET:H	1.73	0.41
1:B:356:ILE:C	1:B:359:PRO:HD2	2.46	0.41
3:D:156:ASN:OD1	3:D:157:GLY:N	2.54	0.41
1:A:138:THR:HG21	1:A:353:PRO:HD2	2.03	0.41
1:B:58:ALA:HA	1:B:61:GLN:HB2	2.02	0.41
2:C:134:PRO:HD2	2:C:196:TRP:CH2	2.56	0.41
1:A:169:LYS:HG2	1:A:170:GLY:N	2.30	0.41
1:A:434:LEU:HD23	1:A:434:LEU:HA	1.97	0.41
1:B:138:THR:HG22	1:B:143:MET:CE	2.45	0.41
1:B:162:VAL:HG23	1:B:166:PHE:CD2	2.55	0.41
1:A:17:ARG:NH1	1:B:119:GLN:HE21	2.19	0.41
1:A:421:LEU:O	1:A:425:MET:HG3	2.21	0.41
1:B:65:MET:SD	1:B:307:PHE:CZ	3.14	0.40
1:B:320:ILE:CG2	1:B:365:THR:HG21	2.51	0.40
3:F:77:MET:SD	3:F:103:LEU:HD21	2.61	0.40
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.22	0.40
1:B:269:PHE:HE1	1:B:341:VAL:HG23	1.87	0.40
1:B:284:HIS:CE1	1:B:291:TRP:CE3	3.09	0.40
1:A:74:ASN:HB2	1:A:77:LEU:CB	2.46	0.40
1:A:445:TYR:OH	4:A:501:CL:CL	2.69	0.40
1:B:298:ILE:C	1:B:298:ILE:CD1	2.94	0.40
2:C:30:SER:C	2:C:32:TYR:H	2.30	0.40
3:F:30:SER:HA	3:F:70:TYR:OH	2.21	0.40
3:F:60:ARG:NH2	3:F:81:ASP:OD1	2.54	0.40
1:B:284:HIS:CE1	1:B:291:TRP:CZ3	3.09	0.40
3:D:141:LYS:HG2	3:D:172:TYR:CG	2.57	0.40
3:D:146:LYS:CB	3:D:194:GLU:HB2	2.51	0.40
3:F:2:ILE:CD1	3:F:92:SER:HB2	2.51	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	442/473 (93%)	424 (96%)	17 (4%)	1 (0%)	43	72
1	B	442/473 (93%)	423 (96%)	18 (4%)	1 (0%)	43	72
2	C	220/222 (99%)	204 (93%)	12 (6%)	4 (2%)	6	25
2	E	219/222 (99%)	203 (93%)	11 (5%)	5 (2%)	5	19
3	D	209/211 (99%)	189 (90%)	16 (8%)	4 (2%)	6	23
3	F	209/211 (99%)	196 (94%)	10 (5%)	3 (1%)	9	30
All	All	1741/1812 (96%)	1639 (94%)	84 (5%)	18 (1%)	12	39

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
2	C	65	LYS
3	D	67	GLY
2	E	65	LYS
2	E	136	SER
3	F	7	SER
1	B	285	GLY
3	D	8	PRO
3	D	76	THR
2	E	64	LEU
3	F	152	SER
2	C	198	SER
2	E	138	ALA
3	F	76	THR
2	C	62	PRO
3	D	142	ASP
1	A	285	GLY
2	E	62	PRO

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	333/356 (94%)	329 (99%)	4 (1%)	63	86
1	B	333/356 (94%)	328 (98%)	5 (2%)	57	84
2	C	182/182 (100%)	182 (100%)	0	100	100
2	E	181/182 (100%)	181 (100%)	0	100	100
3	D	185/185 (100%)	183 (99%)	2 (1%)	65	88
3	F	185/185 (100%)	185 (100%)	0	100	100
All	All	1399/1446 (97%)	1388 (99%)	11 (1%)	73	90

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

Mol	Chain	Res	Type
1	A	18	ARG
1	A	20	GLN
1	A	147	ARG
1	A	442	LYS
1	B	27	GLU
1	B	84	LEU
1	B	163	LEU
1	B	212	LEU
1	B	294	MET
3	D	5	THR
3	D	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	175	HIS
1	B	61	GLN
1	B	153	GLN
1	B	175	HIS
1	B	284	HIS

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Mol	Chain	Res	Type
2	C	39	GLN
3	D	37	GLN
3	D	89	GLN
3	D	165	GLN
2	E	39	GLN
2	E	179	GLN
3	F	37	GLN
3	F	88	GLN
3	F	95	GLN
3	F	165	GLN
3	F	188	HIS

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 3 ligands modelled in this entry, 3 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	444/473 (93%)	0.36	17 (3%) 44 36	79, 107, 149, 234	0
1	B	444/473 (93%)	0.50	35 (7%) 18 15	76, 122, 177, 245	0
2	C	222/222 (100%)	0.30	5 (2%) 61 52	66, 99, 166, 228	0
2	E	221/222 (99%)	0.25	8 (3%) 46 38	65, 96, 142, 242	0
3	D	211/211 (100%)	0.45	13 (6%) 26 21	85, 124, 167, 195	0
3	F	211/211 (100%)	0.16	4 (1%) 66 58	66, 94, 160, 190	0
All	All	1753/1812 (96%)	0.36	82 (4%) 36 28	65, 110, 166, 245	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	GLN	4.7
1	A	234	CYS	4.5
2	E	11	LEU	3.6
2	C	29	TYR	3.5
1	A	230	ARG	3.4
1	B	298	ILE	3.4
2	C	221	ARG	3.4
3	D	7	SER	3.3
1	B	315	GLY	3.3
2	E	4	LEU	3.2
1	B	67	ALA	3.1
2	E	138	ALA	3.1
1	B	163	LEU	3.1
1	B	413	LEU	3.0
3	D	40	GLY	2.9
1	B	377	GLU	2.9
1	A	271	LYS	2.8
1	A	442	LYS	2.8
1	B	125	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	303	GLY	2.8
3	F	186	GLU	2.8
1	B	52	ALA	2.7
3	D	31	TYR	2.7
3	D	163	THR	2.7
1	A	171	ASP	2.6
1	A	400	ALA	2.6
1	B	104	ALA	2.6
3	D	119	PRO	2.6
1	B	210	TYR	2.6
1	B	234	CYS	2.6
1	B	61	GLN	2.6
3	D	17	ASP	2.6
1	A	41	VAL	2.5
1	A	229	TYR	2.5
1	B	396	ALA	2.5
1	B	51	VAL	2.5
1	A	284	HIS	2.5
1	B	66	GLY	2.4
1	B	167	ARG	2.4
1	A	62	ASN	2.4
1	B	18	ARG	2.4
1	A	456	GLN	2.4
1	B	235	GLU	2.4
2	E	84	SER	2.4
2	E	137	ALA	2.4
1	B	302	CYS	2.3
3	D	111	ALA	2.3
3	D	98	GLY	2.3
2	C	128	SER	2.3
1	B	92	PHE	2.3
1	B	438	PHE	2.3
1	B	183	ALA	2.3
3	D	211	ALA	2.2
1	A	71	THR	2.2
1	B	330	MET	2.2
1	B	223	ILE	2.2
1	A	332	MET	2.2
1	A	191	ASN	2.2
1	B	442	LYS	2.2
1	A	210	TYR	2.2
3	F	108	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	173	THR	2.1
2	E	116	THR	2.1
1	B	261	ILE	2.1
2	E	218	ILE	2.1
2	C	202	THR	2.1
1	B	36	LEU	2.1
1	A	169	LYS	2.1
1	B	33	LEU	2.1
1	A	262	PHE	2.1
3	D	5	THR	2.1
1	B	228	MET	2.1
3	D	151	GLY	2.1
3	F	50	THR	2.1
1	B	262	PHE	2.0
3	F	127	GLY	2.0
1	B	54	ASP	2.0
3	D	49	ASP	2.0
3	D	182	LYS	2.0
1	B	236	VAL	2.0
2	E	195	SER	2.0
1	B	324	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($\text{\AA}^2$)	Q<0.9
4	CL	A	502	1/1	0.57	0.45	360,360,360,360	0
4	CL	A	501	1/1	0.93	0.10	114,114,114,114	0

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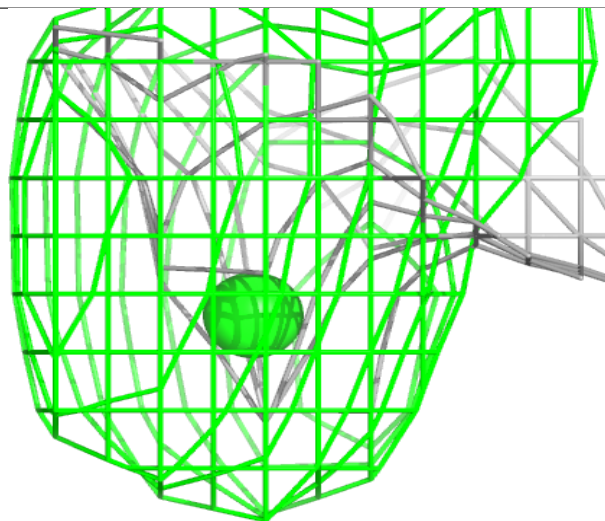
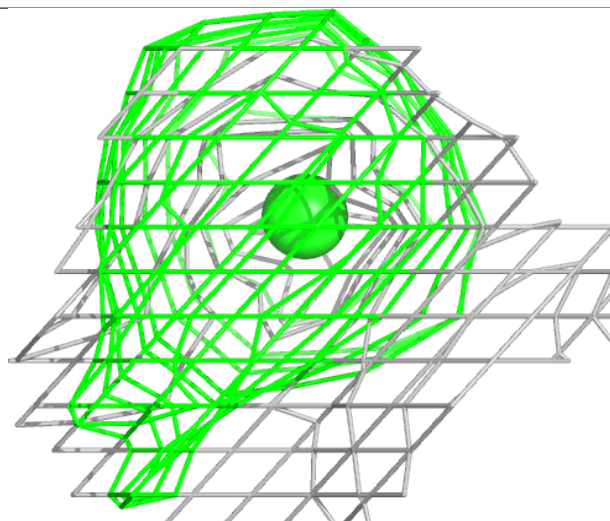
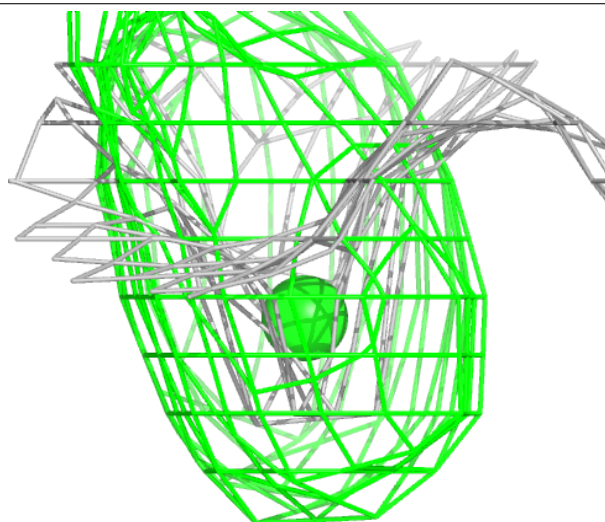
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	501	1/1	0.95	0.22	104,104,104,104	0

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.

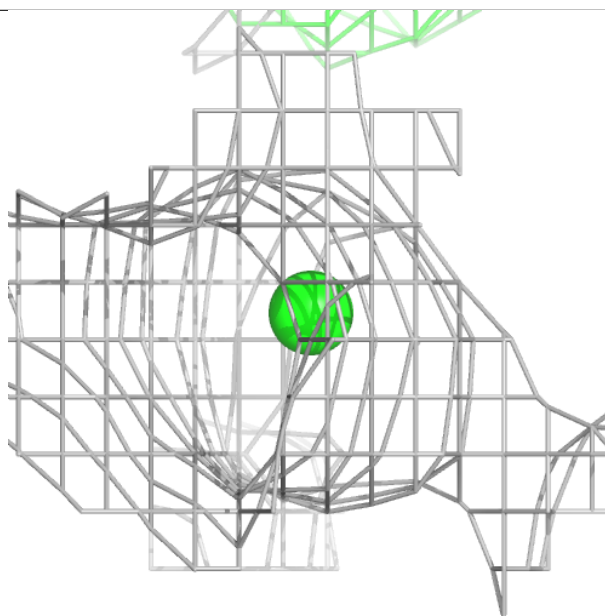
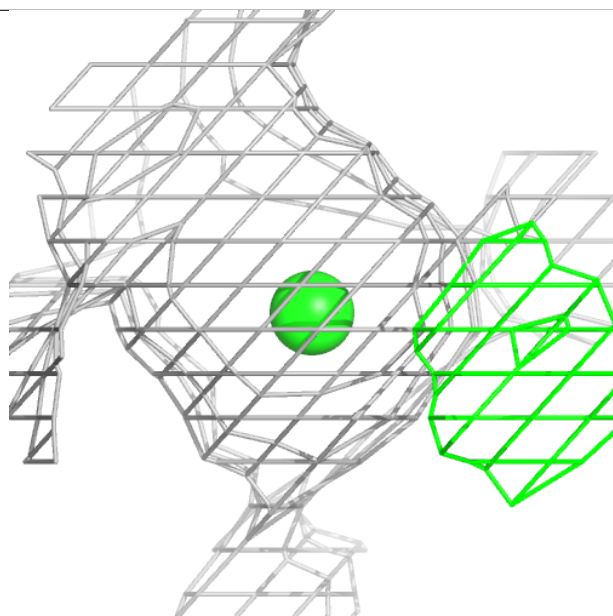
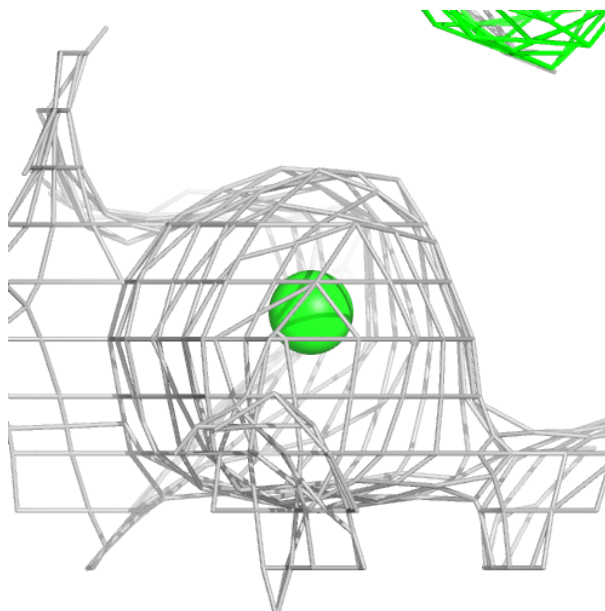
Electron density around CL A 502:

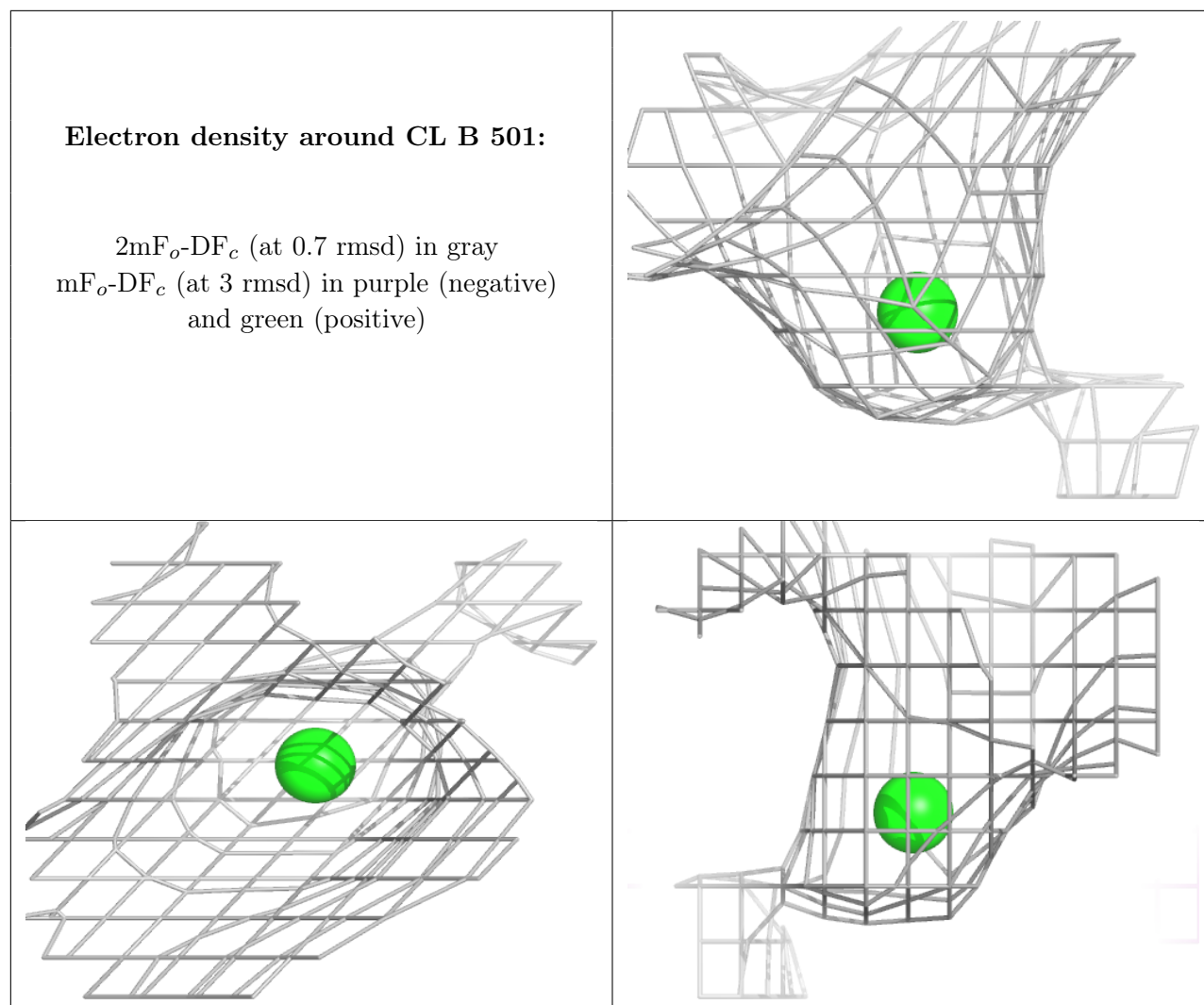
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.