



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:24 AM UTC

PDB ID : 6ADA / pdb_00006ada
Title : Crystal structure of the E148D mutant CLC-ec1 in 200mM bromide
Authors : Lim, H.-H.; Park, K.
Deposited on : 2018-07-31
Resolution : 3.15 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:

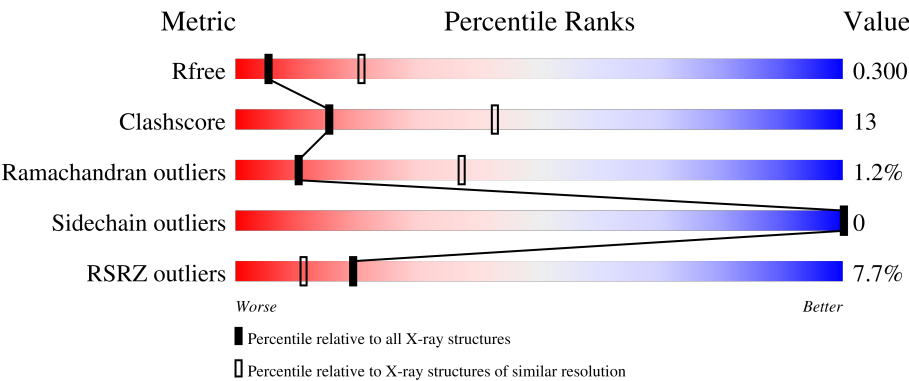
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	7% 67% 26% 6%
1	B	473	12% 63% 30% 7%
2	C	222	4% 76% 23%
2	E	222	4% 71% 27%
3	D	211	8% 62% 36%

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Mol	Chain	Length	Quality of chain
3	F	211	5% 82% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13245 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
			3332	2189	560	563	20			
1	B	442	Total	C	N	O	S	0	0	0
			3314	2179	557	558	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ASP	GLU	engineered mutation	UNP P37019
B	148	ASP	GLU	engineered mutation	UNP P37019

- 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			

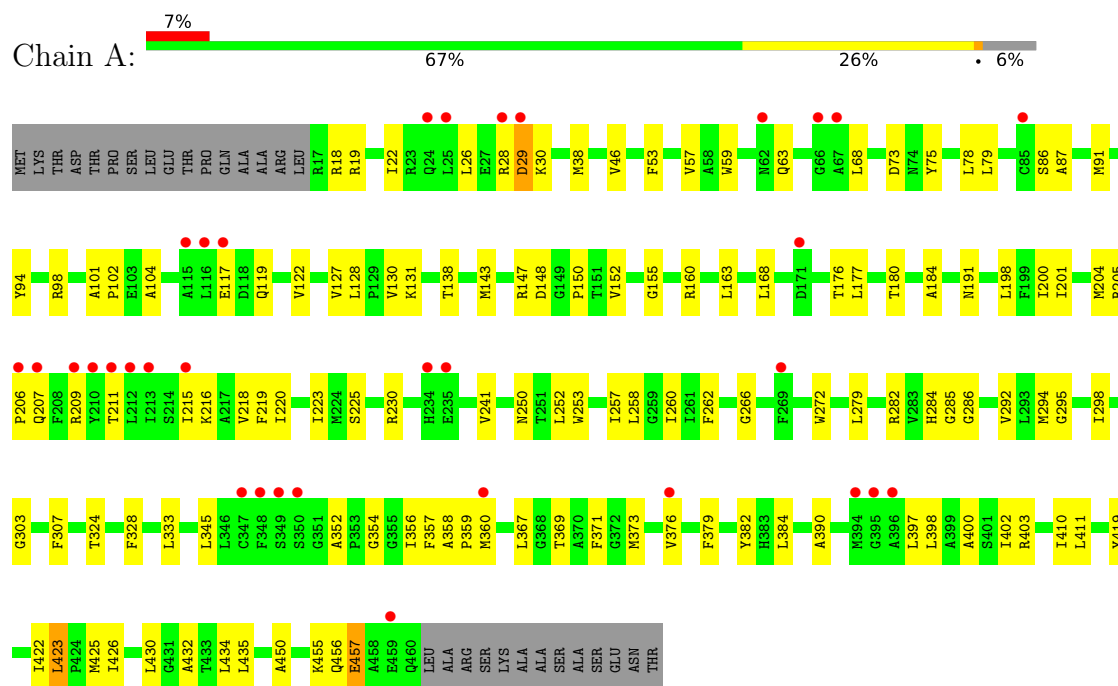
- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

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

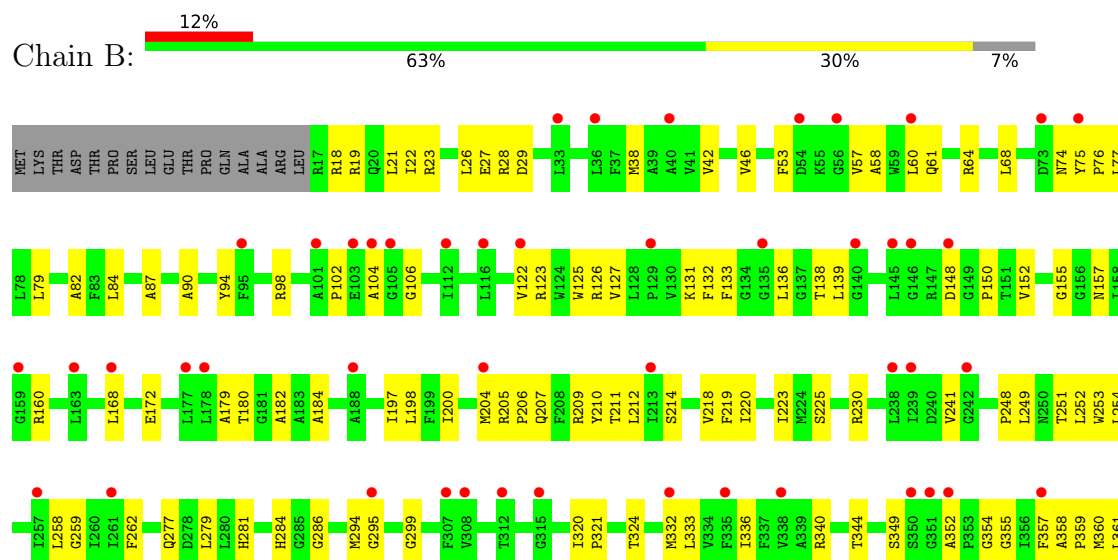
3 Residue-property plots

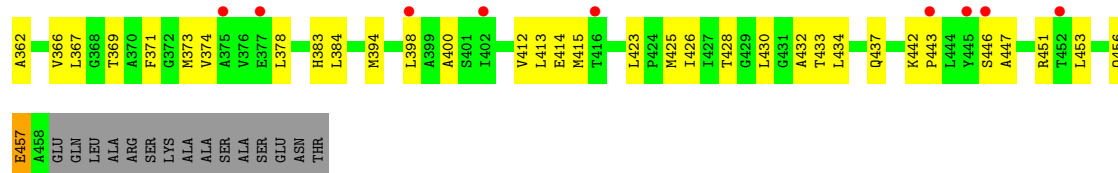
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

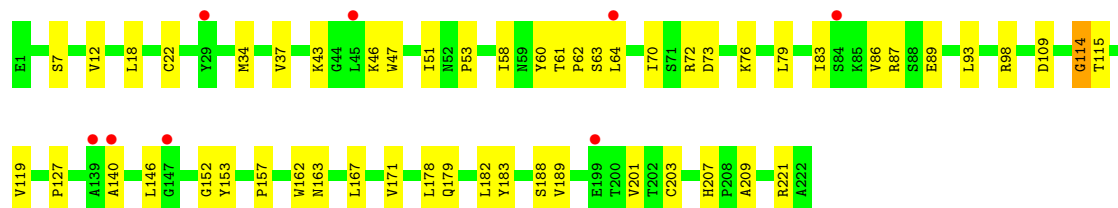
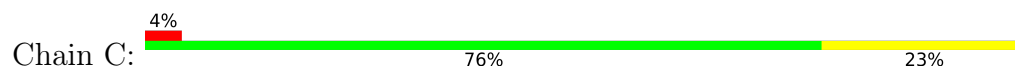


- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

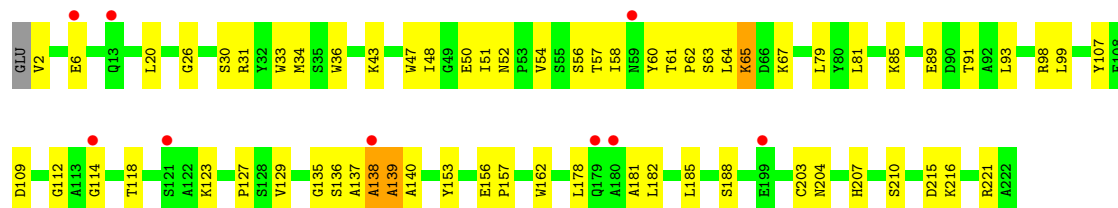




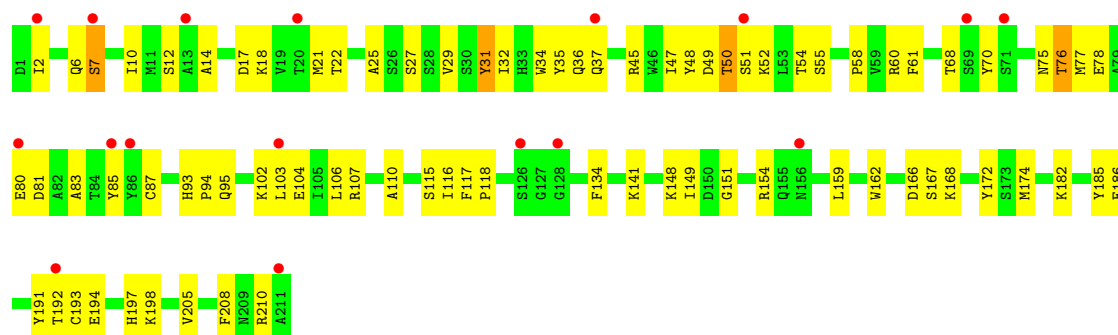
- Molecule 2: antibody Fab fragment, heavy chain



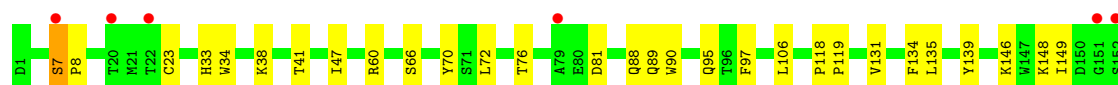
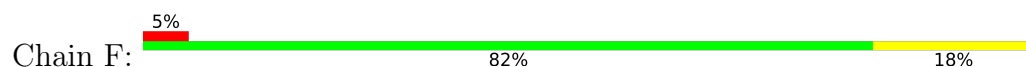
- Molecule 2: antibody Fab fragment, heavy chain

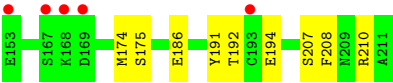


- Molecule 3: antibody Fab fragment, light chain



- 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	232.41Å 99.96Å 170.81Å 90.00° 131.88° 90.00°	Depositor
Resolution (Å)	33.97 – 3.15 33.97 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.97-3.15) 99.4 (33.97-3.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.231 , 0.290 0.235 , 0.300	Depositor DCC
R_{free} test set	2497 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13245	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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

5.1 Standard geometry

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

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	0.42	0/3404	0.69	1/4620 (0.0%)
1	B	0.43	0/3386	0.70	0/4596
2	C	0.52	0/1730	0.75	1/2367 (0.0%)
2	E	0.46	0/1721	0.69	0/2355
3	D	0.49	0/1660	0.75	0/2257
3	F	0.48	0/1660	0.72	0/2257
All	All	0.46	0/13561	0.71	2/18452 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	114	GLY	CA-C-O	-6.35	118.09	122.22
1	A	423	LEU	CB-CG-CD2	-5.13	95.31	110.70

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	3332	0	3482	101	0
1	B	3314	0	3468	117	0
2	C	1681	0	1663	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1672	0	1654	49	0
3	D	1621	0	1546	70	0
3	F	1621	0	1546	30	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
All	All	13245	0	13359	358	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 13.

All (358) 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:194:GLU:HG2	3:D:205:VAL:HG12	1.45	0.99
3:D:95:GLN:OE1	3:D:95:GLN:N	2.05	0.89
3:D:6:GLN:NE2	3:D:85:TYR:O	2.07	0.86
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.62	0.82
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.61	0.81
3:F:89:GLN:O	3:F:95:GLN:HB2	1.82	0.79
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.65	0.77
3:F:186:GLU:O	3:F:210:ARG:NH2	2.18	0.77
3:D:18:LYS:NZ	3:D:75:ASN:OD1	2.17	0.77
3:F:7:SER:OG	3:F:8:PRO:HD3	1.85	0.76
3:D:17:ASP:H	3:D:77:MET:H	1.33	0.75
1:B:172:GLU:HG3	1:B:212:LEU:HB3	1.68	0.75
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.68	0.74
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.68	0.73
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.70	0.73
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.24	0.73
2:E:137:ALA:O	2:E:139:ALA:N	2.21	0.73
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.71	0.72
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.24	0.72
1:A:206:PRO:HD2	1:A:211:THR:HG21	1.72	0.71
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.72	0.71
1:B:106:GLY:O	1:B:131:LYS:NZ	2.23	0.71
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.26	0.70
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.72	0.70
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.74	0.70
1:A:207:GLN:HG2	1:B:28:ARG:HH11	1.56	0.69
3:D:49:ASP:HB2	3:D:52:LYS:HD3	1.73	0.69
3:D:75:ASN:O	3:D:76:THR:HG22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:49:ASP:O	3:D:51:SER:N	2.25	0.69
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.24	0.68
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.75	0.68
1:A:160:ARG:HE	1:A:163:LEU:HD23	1.59	0.68
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.75	0.68
1:A:220:ILE:HD11	1:B:434:LEU:HD11	1.77	0.66
3:F:148:LYS:HB2	3:F:192:THR:HG23	1.77	0.66
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.78	0.66
3:F:95:GLN:H	3:F:95:GLN:CD	2.03	0.66
1:A:430:LEU:HD11	1:B:219:PHE:CD2	2.31	0.65
2:C:163:ASN:HB2	2:C:167:LEU:HD13	1.79	0.65
3:D:25:ALA:O	3:D:68:THR:OG1	2.14	0.65
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.80	0.64
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.31	0.64
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.81	0.63
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.34	0.63
3:D:35:TYR:CD2	3:D:45:ARG:HA	2.33	0.63
1:B:53:PHE:O	1:B:57:VAL:HG23	1.99	0.63
3:D:35:TYR:HD2	3:D:45:ARG:HA	1.64	0.62
1:B:19:ARG:NH1	1:B:19:ARG:HA	2.13	0.62
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.82	0.62
1:B:64:ARG:O	1:B:68:LEU:HG	1.99	0.62
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.00	0.61
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.82	0.61
3:D:29:VAL:CG1	3:D:32:ILE:HD11	2.30	0.61
3:F:47:ILE:HD12	3:F:72:LEU:HD12	1.82	0.61
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.36	0.61
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.83	0.60
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.82	0.60
2:E:135:GLY:O	2:E:137:ALA:N	2.30	0.60
2:E:61:THR:O	2:E:63:SER:N	2.34	0.60
1:B:180:THR:HG22	1:B:218:VAL:HA	1.83	0.60
3:D:7:SER:HB3	3:D:22:THR:HB	1.82	0.60
1:A:357:PHE:HE1	1:A:411:LEU:HD22	1.66	0.60
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.37	0.60
1:A:18:ARG:NH1	1:B:456:GLN:O	2.35	0.59
3:D:29:VAL:O	3:D:70:TYR:OH	2.19	0.59
3:D:36:GLN:HB2	3:D:85:TYR:CE1	2.37	0.59
1:A:160:ARG:NE	1:A:163:LEU:HD23	2.16	0.59
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.84	0.59
1:A:28:ARG:HH11	1:B:207:GLN:HG2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.85	0.59
1:A:250:ASN:ND2	1:A:382:TYR:HE1	2.01	0.59
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.84	0.59
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.85	0.58
2:E:47:TRP:CD2	3:F:95:GLN:NE2	2.72	0.58
1:A:147:ARG:HD2	4:A:501:BR:BR	2.59	0.58
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.85	0.57
1:B:262:PHE:CE2	1:B:367:LEU:HD23	2.39	0.57
1:A:430:LEU:HD11	1:B:219:PHE:CG	2.39	0.57
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.85	0.57
1:A:73:ASP:N	1:A:73:ASP:OD1	2.36	0.57
2:C:60:TYR:HE1	2:C:70:ILE:HG13	1.70	0.57
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.85	0.57
1:A:201:ILE:HD11	1:A:215:ILE:HD13	1.86	0.57
3:D:31:TYR:HA	3:D:50:THR:OG1	2.05	0.57
1:A:53:PHE:O	1:A:57:VAL:HG23	2.05	0.56
1:A:180:THR:HB	1:A:218:VAL:HA	1.88	0.56
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.85	0.56
1:B:42:VAL:O	1:B:46:VAL:HG23	2.06	0.56
1:A:94:TYR:CE1	1:A:295:GLY:HA3	2.41	0.56
3:F:95:GLN:CD	3:F:95:GLN:N	2.64	0.56
2:C:7:SER:HA	2:C:115:THR:HG21	1.86	0.56
3:F:135:LEU:HD13	3:F:174:MET:HE2	1.88	0.56
1:B:19:ARG:HA	1:B:19:ARG:CZ	2.36	0.55
2:E:2:VAL:HA	2:E:26:GLY:HA3	1.88	0.55
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.86	0.55
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.35	0.55
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.88	0.55
3:D:162:TRP:NE1	3:D:174:MET:HG3	2.21	0.55
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.28	0.55
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.40	0.55
1:A:423:LEU:CD1	1:B:230:ARG:CZ	2.85	0.55
3:D:95:GLN:H	3:D:95:GLN:CD	2.11	0.54
3:D:149:ILE:HG12	3:D:191:TYR:CD2	2.43	0.54
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.88	0.54
1:B:209:ARG:HG3	1:B:210:TYR:O	2.08	0.54
1:B:430:LEU:HA	1:B:433:THR:HG22	1.90	0.54
2:C:178:LEU:HB2	2:C:183:TYR:CE1	2.43	0.54
2:C:152:GLY:C	2:C:182:LEU:HD22	2.33	0.54
1:A:219:PHE:HE1	1:B:426:ILE:HG23	1.73	0.53
3:D:36:GLN:HB2	3:D:85:TYR:HE1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:MET:HE3	1:A:298:ILE:HG22	1.90	0.53
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.42	0.53
2:E:52:ASN:ND2	2:E:57:THR:H	2.06	0.53
3:D:191:TYR:HB2	3:D:208:PHE:CE1	2.43	0.53
3:F:95:GLN:N	3:F:95:GLN:OE1	2.26	0.53
1:B:206:PRO:CG	1:B:211:THR:HG21	2.38	0.53
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.90	0.53
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.91	0.52
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.91	0.52
1:A:456:GLN:O	1:B:18:ARG:NH1	2.43	0.52
2:E:156:GLU:OE1	2:E:157:PRO:HA	2.09	0.52
1:A:455:LYS:C	1:A:457:GLU:H	2.17	0.52
2:E:207:HIS:ND1	2:E:210:SER:OG	2.41	0.52
1:A:328:PHE:O	1:A:373:MET:HE1	2.10	0.52
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.40	0.52
2:E:47:TRP:CG	3:F:95:GLN:NE2	2.78	0.52
3:F:90:TRP:CD1	3:F:95:GLN:HB3	2.45	0.52
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.40	0.52
1:A:177:LEU:HA	1:A:180:THR:CG2	2.40	0.52
1:A:423:LEU:HD13	1:B:230:ARG:CZ	2.40	0.52
1:B:413:LEU:HD13	1:B:425:MET:HE1	1.92	0.52
2:E:138:ALA:O	2:E:140:ALA:N	2.43	0.52
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.91	0.51
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.91	0.51
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.92	0.51
3:D:17:ASP:OD1	3:D:18:LYS:N	2.43	0.51
3:D:77:MET:HE3	3:D:78:GLU:O	2.10	0.51
1:A:379:PHE:HB3	1:A:382:TYR:CD2	2.46	0.51
2:C:162:TRP:CZ3	2:C:203:CYS:HB2	2.46	0.51
3:F:60:ARG:NH2	3:F:81:ASP:OD1	2.45	0.50
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.25	0.50
1:A:333:LEU:HD11	1:A:369:THR:HG22	1.93	0.50
1:B:279:LEU:O	1:B:279:LEU:HD23	2.10	0.50
3:D:12:SER:HA	3:D:104:GLU:O	2.11	0.50
2:E:135:GLY:C	2:E:137:ALA:H	2.18	0.50
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.47	0.50
2:E:91:THR:HG23	2:E:118:THR:HA	1.94	0.50
1:B:38:MET:O	1:B:42:VAL:HG23	2.12	0.50
2:C:163:ASN:HD21	2:C:201:VAL:HA	1.77	0.50
1:B:94:TYR:CE1	1:B:295:GLY:HA3	2.47	0.49
1:A:284:HIS:C	1:A:286:GLY:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:TRP:CE2	3:D:174:MET:HG3	2.47	0.49
1:A:184:ALA:HB1	1:A:225:SER:CB	2.38	0.49
1:B:383:HIS:NE2	2:E:50:GLU:OE1	2.41	0.49
1:A:29:ASP:OD1	1:A:216:LYS:HE3	2.12	0.49
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.47	0.49
1:B:249:LEU:C	1:B:251:THR:H	2.21	0.49
2:E:221:ARG:NH2	3:F:118:PRO:HD2	2.28	0.49
2:C:93:LEU:HD11	2:C:114:GLY:HA3	1.95	0.49
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.48	0.49
3:D:185:TYR:CZ	3:D:210:ARG:HD3	2.48	0.49
2:E:188:SER:HB2	3:F:134:PHE:CE2	2.48	0.49
1:B:132:PHE:O	1:B:136:LEU:HG	2.12	0.49
1:B:148:ASP:OD2	1:B:355:GLY:HA3	2.13	0.49
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.94	0.49
3:D:34:TRP:CH2	3:D:87:CYS:HB3	2.48	0.49
1:B:184:ALA:HB1	1:B:225:SER:CB	2.42	0.48
3:D:106:LEU:HD23	3:D:107:ARG:N	2.28	0.48
3:D:110:ALA:O	3:D:197:HIS:HE1	1.96	0.48
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.95	0.48
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.48	0.48
1:B:374:VAL:O	1:B:378:LEU:HG	2.13	0.48
3:D:141:LYS:HD3	3:D:172:TYR:CE1	2.49	0.48
1:A:241:VAL:HG21	1:A:324:THR:HG21	1.96	0.48
3:D:166:ASP:OD1	3:D:167:SER:N	2.46	0.48
1:A:86:SER:OG	1:A:303:GLY:HA3	2.14	0.48
1:A:148:ASP:CG	1:A:357:PHE:HB2	2.39	0.48
1:A:160:ARG:HA	1:A:160:ARG:HD2	1.64	0.48
3:D:49:ASP:C	3:D:51:SER:H	2.21	0.48
1:A:219:PHE:CE1	1:B:426:ILE:HG23	2.49	0.47
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.49	0.47
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.96	0.47
2:C:146:LEU:HB2	2:C:189:VAL:HG12	1.96	0.47
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.96	0.47
3:D:58:PRO:HG2	3:D:61:PHE:CE2	2.49	0.47
3:D:149:ILE:HG23	3:D:191:TYR:CE2	2.49	0.47
1:B:160:ARG:HA	1:B:160:ARG:HD2	1.72	0.47
1:B:22:ILE:O	1:B:26:LEU:HD12	2.14	0.47
2:C:73:ASP:OD2	2:C:76:LYS:HD2	2.15	0.47
3:D:48:TYR:O	3:D:52:LYS:HB2	2.14	0.47
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.40	0.47
2:E:67:LYS:NZ	2:E:85:LYS:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:O	1:B:79:LEU:HG	2.14	0.47
2:E:204:ASN:ND2	2:E:215:ASP:OD1	2.48	0.47
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.95	0.46
2:E:34:MET:HB2	2:E:79:LEU:HD13	1.97	0.46
1:B:248:PRO:O	1:B:251:THR:HB	2.16	0.46
2:C:37:VAL:HG13	2:C:46:LYS:O	2.14	0.46
3:D:50:THR:HG22	3:D:51:SER:OG	2.15	0.46
3:D:58:PRO:HG2	3:D:61:PHE:HE2	1.80	0.46
1:A:403:ARG:NH2	1:B:29:ASP:O	2.49	0.46
3:D:29:VAL:HG12	3:D:32:ILE:HD11	1.96	0.46
3:F:34:TRP:HB2	3:F:47:ILE:HB	1.97	0.46
1:A:59:TRP:O	1:A:63:GLN:HG2	2.15	0.46
1:B:258:LEU:HD23	1:B:428:THR:HG21	1.98	0.46
2:C:179:GLN:NE2	3:D:159:LEU:HD11	2.30	0.46
3:D:197:HIS:CG	3:D:198:LYS:H	2.33	0.46
3:F:186:GLU:HA	3:F:210:ARG:CZ	2.45	0.46
1:B:60:LEU:O	1:B:64:ARG:HG3	2.15	0.46
1:B:214:SER:O	1:B:218:VAL:HG23	2.15	0.46
1:A:148:ASP:O	1:A:152:VAL:HG23	2.16	0.46
1:B:369:THR:O	1:B:373:MET:HG3	2.16	0.46
2:C:18:LEU:HD11	2:C:83:ILE:HD12	1.98	0.46
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.98	0.46
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.84	0.46
1:B:148:ASP:CG	1:B:357:PHE:HB2	2.41	0.46
1:B:253:TRP:CZ2	1:B:254:LEU:HD21	2.51	0.46
1:A:122:VAL:HG11	1:A:160:ARG:HB2	1.97	0.45
1:B:253:TRP:CH2	1:B:254:LEU:HD21	2.51	0.45
1:B:84:LEU:HA	1:B:87:ALA:HB3	1.98	0.45
2:E:89:GLU:N	2:E:89:GLU:OE1	2.49	0.45
2:E:98:ARG:O	2:E:109:ASP:HB3	2.16	0.45
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.97	0.45
2:E:58:ILE:HG22	2:E:60:TYR:CE2	2.52	0.45
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.99	0.45
2:E:54:VAL:C	2:E:56:SER:H	2.25	0.45
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.49	0.45
3:D:34:TRP:CZ3	3:D:87:CYS:HB3	2.51	0.45
1:A:419:TYR:CZ	1:B:414:GLU:HG2	2.52	0.45
1:B:200:ILE:HD11	1:B:204:MET:HE2	1.97	0.45
2:C:43:LYS:HE2	2:C:43:LYS:HB3	1.43	0.45
1:A:266:GLY:HA3	1:A:400:ALA:HB1	1.99	0.45
2:C:61:THR:O	2:C:63:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:MET:HG2	3:D:78:GLU:N	2.32	0.45
1:A:87:ALA:O	1:A:91:MET:HG3	2.18	0.44
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.99	0.44
1:A:68:LEU:HD13	1:A:307:PHE:CD2	2.52	0.44
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.33	0.44
1:B:294:MET:HE2	1:B:294:MET:HB3	1.66	0.44
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.53	0.44
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.52	0.44
1:B:38:MET:HG3	1:B:168:LEU:HD11	2.00	0.44
1:B:277:GLN:HG2	1:B:349:SER:HA	1.99	0.44
1:B:332:MET:O	1:B:336:ILE:HG13	2.18	0.44
1:B:361:LEU:HD13	1:B:415:MET:HE1	2.00	0.44
1:A:91:MET:HG2	1:A:292:VAL:O	2.17	0.44
1:B:46:VAL:HG22	1:B:155:GLY:HA2	2.00	0.44
1:A:30:LYS:HA	1:B:437:GLN:CD	2.42	0.44
1:A:200:ILE:HD11	1:A:204:MET:HE2	1.99	0.44
3:D:14:ALA:O	3:D:17:ASP:HB3	2.17	0.44
1:A:223:ILE:HD11	1:B:426:ILE:HG22	2.00	0.44
1:A:253:TRP:O	1:A:257:ILE:HG13	2.17	0.44
1:A:272:TRP:HE3	1:A:345:LEU:HD11	1.83	0.44
1:A:422:ILE:HA	1:A:425:MET:HE3	2.00	0.44
1:B:394:MET:HE2	1:B:412:VAL:HG22	1.99	0.44
2:C:188:SER:HB2	3:D:134:PHE:CE2	2.52	0.44
3:D:149:ILE:HG12	3:D:191:TYR:HD2	1.83	0.44
1:A:360:MET:HE1	1:A:402:ILE:HG23	2.00	0.44
3:D:21:MET:SD	3:D:85:TYR:HB2	2.58	0.44
3:F:38:LYS:O	3:F:41:THR:HB	2.17	0.44
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.48	0.43
1:A:104:ALA:O	1:A:131:LYS:NZ	2.41	0.43
1:A:430:LEU:HD23	1:B:220:ILE:HG12	1.99	0.43
1:A:369:THR:O	1:A:373:MET:HG3	2.18	0.43
1:B:284:HIS:C	1:B:286:GLY:H	2.25	0.43
3:D:116:ILE:HD12	3:D:193:CYS:HB3	2.00	0.43
2:E:85:LYS:HA	2:E:85:LYS:HD3	1.86	0.43
3:F:119:PRO:HD3	3:F:131:VAL:HG22	2.00	0.43
1:B:241:VAL:HG21	1:B:324:THR:HG21	2.00	0.43
1:A:177:LEU:HA	1:A:180:THR:HG22	2.01	0.43
2:C:12:VAL:HG21	2:C:18:LEU:HD23	2.00	0.43
2:E:52:ASN:HD21	2:E:56:SER:HB3	1.83	0.43
2:E:64:LEU:HB3	2:E:65:LYS:H	1.63	0.43
3:F:149:ILE:HG12	3:F:191:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:O	1:A:180:THR:HG22	2.19	0.43
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.82	0.43
3:F:66:SER:HA	3:F:70:TYR:CZ	2.53	0.43
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.37	0.43
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.54	0.43
3:D:115:SER:HB3	3:D:117:PHE:CE1	2.53	0.43
3:D:149:ILE:HD12	3:D:154:ARG:HH11	1.82	0.43
1:A:26:LEU:HD22	1:B:442:LYS:HE3	2.01	0.43
1:A:127:VAL:O	1:A:128:LEU:C	2.61	0.43
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.54	0.43
1:B:23:ARG:HH21	1:B:27:GLU:HG3	1.83	0.43
1:B:68:LEU:HD21	1:B:82:ALA:HB2	2.00	0.43
2:E:30:SER:O	2:E:31:ARG:HB2	2.19	0.42
1:B:453:LEU:O	1:B:457:GLU:HG2	2.18	0.42
3:D:6:GLN:HA	3:D:22:THR:O	2.19	0.42
2:E:178:LEU:HD12	2:E:182:LEU:O	2.19	0.42
1:B:58:ALA:HA	1:B:61:GLN:OE1	2.19	0.42
1:B:252:LEU:HD11	1:B:423:LEU:HD23	2.01	0.42
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.72	0.42
2:E:129:VAL:O	2:E:216:LYS:HE3	2.19	0.42
1:B:259:GLY:N	1:B:428:THR:HG23	2.34	0.42
2:E:6:GLU:OE1	2:E:112:GLY:HA3	2.18	0.42
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.49	0.42
3:D:54:THR:HG22	3:D:55:SER:N	2.34	0.42
1:A:119:GLN:HG3	1:B:21:LEU:HD23	2.02	0.42
3:F:192:THR:HB	3:F:207:SER:HB3	2.01	0.42
1:A:205:ARG:HH12	1:B:205:ARG:HH12	1.68	0.42
1:B:333:LEU:HD11	1:B:369:THR:HG22	2.02	0.42
2:C:87:ARG:NH2	2:C:89:GLU:OE1	2.38	0.42
2:C:86:VAL:HG12	2:C:119:VAL:HG21	2.02	0.42
2:E:52:ASN:HD21	2:E:57:THR:H	1.65	0.42
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.54	0.42
1:A:426:ILE:HG22	1:B:223:ILE:HD11	2.02	0.42
1:B:122:VAL:HG11	1:B:160:ARG:HB2	2.02	0.42
3:D:37:GLN:O	3:D:83:ALA:HB1	2.20	0.42
1:B:133:PHE:HA	1:B:136:LEU:HD12	2.02	0.41
2:E:123:LYS:HB3	2:E:123:LYS:HE2	1.80	0.41
1:A:369:THR:OG1	1:A:390:ALA:HB2	2.20	0.41
2:C:127:PRO:HB3	2:C:153:TYR:HB3	2.02	0.41
3:D:10:ILE:HG23	3:D:102:LYS:HB3	2.01	0.41
3:F:106:LEU:HA	3:F:139:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.55	0.41
1:B:123:ARG:O	1:B:127:VAL:HG23	2.20	0.41
1:B:383:HIS:HD2	2:E:33:TRP:CZ3	2.37	0.41
2:E:20:LEU:N	2:E:81:LEU:O	2.52	0.41
1:A:19:ARG:HA	1:A:22:ILE:HD12	2.01	0.41
1:A:216:LYS:NZ	1:B:433:THR:O	2.54	0.41
1:A:279:LEU:HA	1:A:282:ARG:HH11	1.86	0.41
1:A:294:MET:HE2	1:A:294:MET:HB3	1.77	0.41
1:A:356:ILE:HG23	1:A:360:MET:HE2	2.03	0.41
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.81	0.41
3:D:80:GLU:H	3:D:80:GLU:HG2	1.60	0.41
2:E:185:LEU:C	2:E:185:LEU:HD12	2.45	0.41
1:A:376:VAL:HG22	1:A:384:LEU:HB2	2.02	0.41
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.36	0.41
1:B:200:ILE:CD1	1:B:204:MET:HE2	2.51	0.41
2:C:51:ILE:HD13	2:C:72:ARG:HG2	2.02	0.41
3:D:93:HIS:CG	3:D:94:PRO:HA	2.54	0.41
2:E:93:LEU:HD11	2:E:114:GLY:HA3	2.03	0.41
3:F:174:MET:HG2	3:F:175:SER:N	2.34	0.41
1:A:219:PHE:CG	1:B:430:LEU:HD11	2.56	0.41
3:D:29:VAL:HG11	3:D:32:ILE:HD11	2.00	0.41
2:E:99:LEU:HD23	2:E:99:LEU:HA	1.85	0.41
1:B:179:ALA:O	1:B:182:ALA:N	2.53	0.41
1:B:362:ALA:O	1:B:366:VAL:HG23	2.20	0.41
3:D:148:LYS:HB3	3:D:151:GLY:HA2	2.03	0.41
2:E:178:LEU:HD11	2:E:181:ALA:HA	2.02	0.41
3:F:191:TYR:HB2	3:F:208:PHE:CE1	2.55	0.41
1:B:340:ARG:O	1:B:344:THR:OG1	2.26	0.41
3:D:77:MET:SD	3:D:103:LEU:HD21	2.61	0.41
1:A:46:VAL:HG22	1:A:155:GLY:HA2	2.03	0.40
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.90	0.40
2:E:36:TRP:O	2:E:48:ILE:HB	2.21	0.40
3:F:23:CYS:N	3:F:70:TYR:O	2.26	0.40
1:B:204:MET:HE3	1:B:204:MET:HB3	1.75	0.40
1:B:447:ALA:O	1:B:451:ARG:HG3	2.21	0.40
1:A:19:ARG:HB3	1:A:19:ARG:CZ	2.51	0.40
1:B:197:ILE:HD11	1:B:219:PHE:CE1	2.55	0.40
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.56	0.40
1:B:57:VAL:CG1	1:B:139:LEU:HB3	2.52	0.40
3:D:182:LYS:O	3:D:186:GLU:HG3	2.22	0.40
3:D:186:GLU:HA	3:D:210:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:LYS:HB3	2:E:43:LYS:HE2	1.83	0.40
2:E:54:VAL:C	2:E:56:SER:N	2.79	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	442/473 (93%)	409 (92%)	29 (7%)	4 (1%)	14	43
1	B	440/473 (93%)	408 (93%)	31 (7%)	1 (0%)	43	71
2	C	220/222 (99%)	197 (90%)	19 (9%)	4 (2%)	6	29
2	E	219/222 (99%)	196 (90%)	18 (8%)	5 (2%)	5	24
3	D	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	4	23
3	F	209/211 (99%)	196 (94%)	11 (5%)	2 (1%)	12	41
All	All	1739/1812 (96%)	1593 (92%)	125 (7%)	21 (1%)	10	37

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	62	PRO
2	E	138	ALA
2	E	139	ALA
2	C	140	ALA
3	D	31	TYR
3	D	76	THR
2	E	65	LYS
2	E	136	SER
1	A	29	ASP
2	C	64	LEU

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Mol	Chain	Res	Type
3	D	50	THR
3	D	168	LYS
3	F	7	SER
1	B	457	GLU
3	F	76	THR
1	A	457	GLU
2	C	62	PRO
1	A	450	ALA
3	D	7	SER
1	A	285	GLY
2	C	157	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/358 (94%)	335 (100%)	0	100	100
1	B	333/358 (93%)	333 (100%)	0	100	100
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%)	185 (100%)	0	100	100
3	F	185/185 (100%)	185 (100%)	0	100	100
All	All	1401/1450 (97%)	1401 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	61	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN

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Mol	Chain	Res	Type
1	A	281	HIS
1	B	20	GLN
1	B	119	GLN
1	B	207	GLN
1	B	270	ASN
1	B	284	HIS
1	B	437	GLN
2	C	163	ASN
3	D	136	ASN
3	D	137	ASN
2	E	82	GLN
2	E	172	HIS
3	F	36	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.49	33 (7%) 20 12	64, 95, 122, 154	0
1	B	442/473 (93%)	0.92	56 (12%) 8 5	68, 98, 130, 162	0
2	C	222/222 (100%)	0.37	8 (3%) 46 27	55, 83, 117, 147	0
2	E	221/222 (99%)	0.23	9 (4%) 41 24	54, 81, 116, 150	0
3	D	211/211 (100%)	0.64	17 (8%) 18 10	68, 93, 115, 122	0
3	F	211/211 (100%)	0.22	11 (5%) 33 19	55, 76, 129, 139	0
All	All	1751/1812 (96%)	0.54	134 (7%) 19 11	54, 91, 124, 162	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	GLU	6.8
1	B	239	ILE	6.4
1	A	211	THR	5.4
1	B	104	ALA	5.4
1	B	148	ASP	5.0
1	A	209	ARG	4.8
1	A	213	ILE	4.8
1	B	238	LEU	4.8
1	B	307	PHE	4.6
3	F	167	SER	4.6
1	B	159	GLY	4.2
1	A	394	MET	4.2
1	B	73	ASP	4.2
1	B	163	LEU	4.1
1	A	66	GLY	4.1
1	A	376	VAL	4.0
1	B	40	ALA	3.9
1	B	312	THR	3.8
1	B	402	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	395	GLY	3.8
1	A	396	ALA	3.8
1	A	234	HIS	3.8
3	F	7	SER	3.7
1	B	375	ALA	3.7
1	A	348	PHE	3.6
2	E	59	ASN	3.6
1	A	347	CYS	3.5
1	B	95	PHE	3.5
1	B	122	VAL	3.4
1	B	105	GLY	3.4
2	E	180	ALA	3.4
1	A	25	LEU	3.4
3	D	80	GLU	3.3
1	B	357	PHE	3.3
1	B	261	ILE	3.3
3	D	7	SER	3.3
1	A	67	ALA	3.2
1	B	335	PHE	3.2
2	E	13	GLN	3.2
3	D	103	LEU	3.2
1	A	29	ASP	3.1
1	B	308	VAL	3.1
1	B	145	LEU	3.1
1	A	350	SER	3.1
2	C	29	TYR	3.1
3	D	71	SER	3.1
3	D	211	ALA	3.0
2	C	199	GLU	3.0
2	E	179	GLN	3.0
1	A	212	LEU	3.0
1	B	177	LEU	3.0
1	B	315	GLY	3.0
1	A	117	GLU	2.9
1	A	28	ARG	2.9
3	F	168	LYS	2.9
1	A	207	GLN	2.9
1	A	349	SER	2.8
3	D	156	ASN	2.8
2	C	84	SER	2.8
2	E	138	ALA	2.8
1	A	360	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	235	GLU	2.8
3	D	86	TYR	2.8
1	B	350	SER	2.8
3	F	193	CYS	2.8
1	A	116	LEU	2.8
1	A	459	GLU	2.8
1	A	206	PRO	2.7
3	D	192	THR	2.7
1	B	56	GLY	2.7
2	C	139	ALA	2.7
1	B	112	ILE	2.7
1	B	146	GLY	2.7
3	D	128	GLY	2.6
3	F	153	GLU	2.6
3	F	152	SER	2.6
1	A	269	PHE	2.6
2	C	147	GLY	2.6
1	B	338	VAL	2.6
3	D	13	ALA	2.6
2	E	121	SER	2.5
1	B	54	ASP	2.5
1	B	416	THR	2.5
1	B	351	GLY	2.5
1	B	242	GLY	2.5
1	A	85	CYS	2.5
1	A	210	TYR	2.5
2	E	6	GLU	2.4
1	B	33	LEU	2.4
3	F	20	THR	2.4
1	B	101	ALA	2.4
1	B	332	MET	2.4
3	D	69	SER	2.4
3	D	126	SER	2.4
1	B	295	GLY	2.4
3	F	151	GLY	2.4
1	B	178	LEU	2.4
1	A	215	ILE	2.3
1	A	62	ASN	2.3
2	E	199	GLU	2.3
3	D	20	THR	2.2
1	B	445	TYR	2.2
3	D	85	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	2	ILE	2.2
1	B	352	ALA	2.2
1	B	213	ILE	2.2
1	B	116	LEU	2.2
1	B	168	LEU	2.2
1	A	115	ALA	2.2
1	A	171	ASP	2.2
1	B	75	TYR	2.2
1	B	257	ILE	2.2
1	B	398	LEU	2.2
1	B	135	GLY	2.2
2	E	114	GLY	2.2
1	B	204	MET	2.1
2	C	140	ALA	2.1
1	B	446	SER	2.1
2	C	64	LEU	2.1
3	D	51	SER	2.1
1	B	188	ALA	2.1
1	A	24	GLN	2.1
1	B	140	GLY	2.1
2	C	45	LEU	2.1
3	F	169	ASP	2.1
1	B	452	THR	2.1
1	B	443	PRO	2.1
3	F	22	THR	2.0
1	B	129	PRO	2.0
1	B	103	GLU	2.0
3	F	79	ALA	2.0
3	D	37	GLN	2.0
1	B	36	LEU	2.0
1	B	60	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 oligosaccharides in this entry.

6.4 Ligands

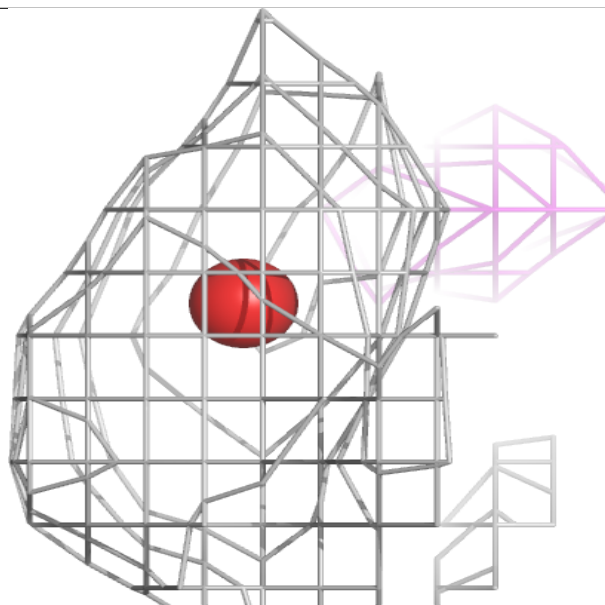
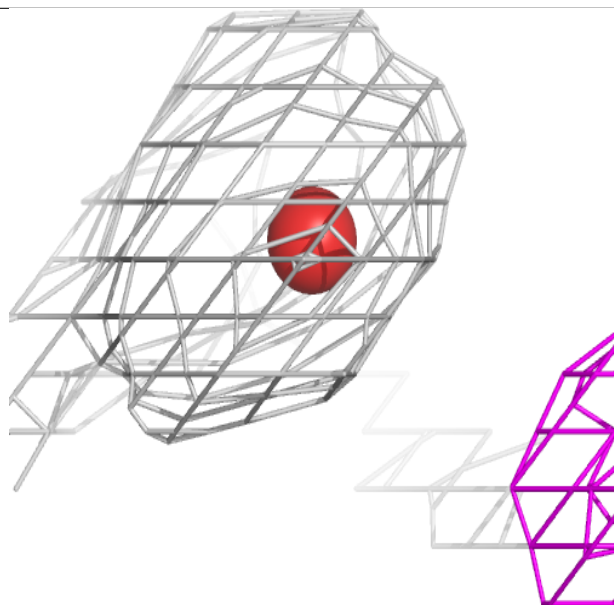
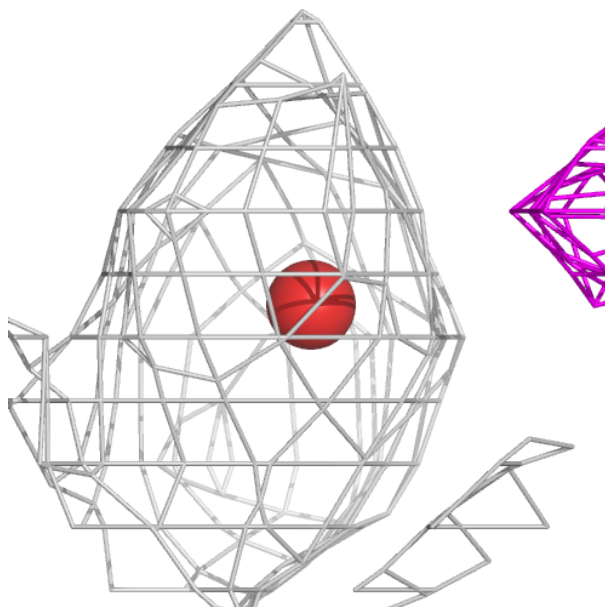
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BR	B	501	1/1	0.80	0.29	195,195,195,195	0
4	BR	B	502	1/1	0.86	0.12	133,133,133,133	0
4	BR	A	501	1/1	0.88	0.22	174,174,174,174	0
4	BR	A	502	1/1	0.94	0.15	159,159,159,159	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.

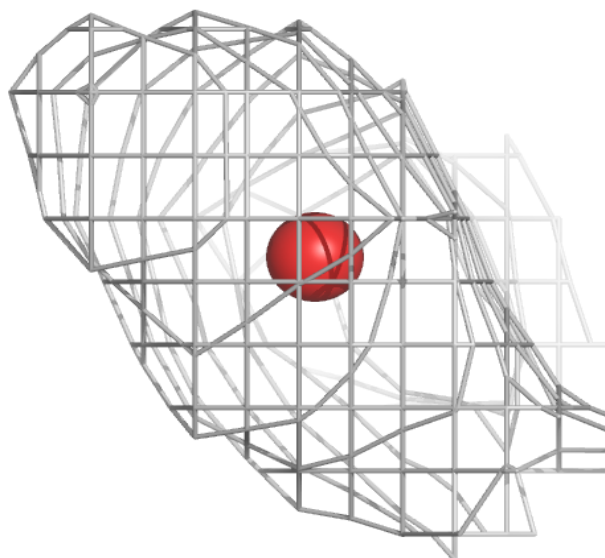
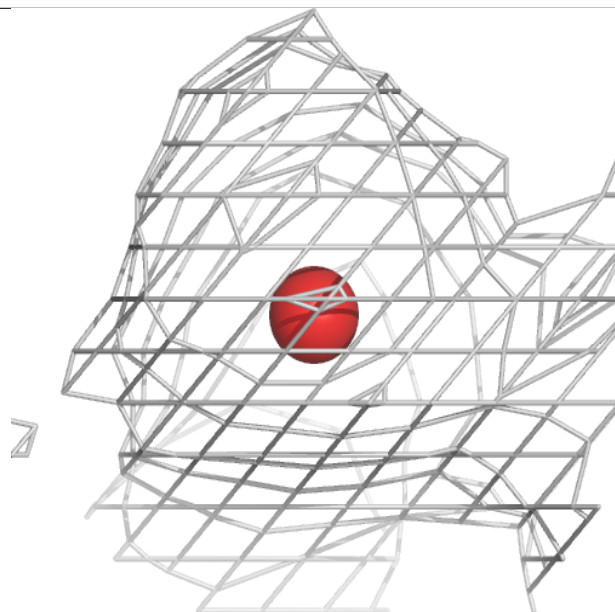
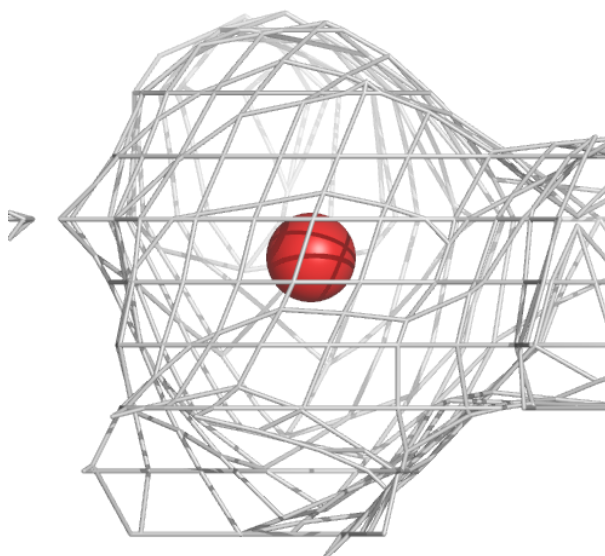
Electron density around BR B 501:

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



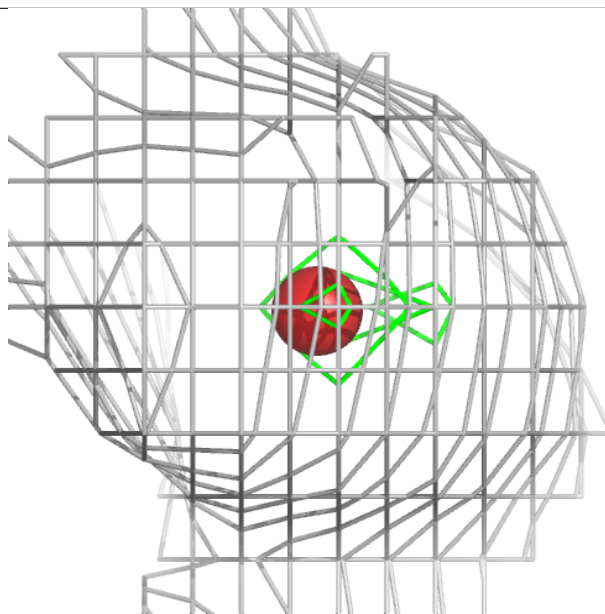
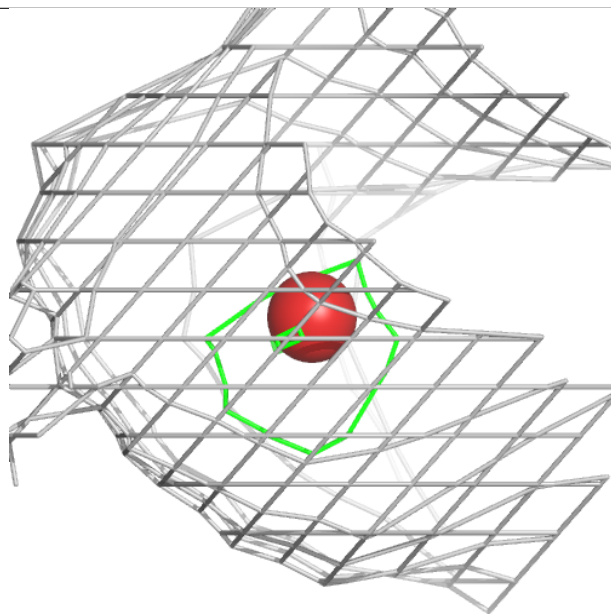
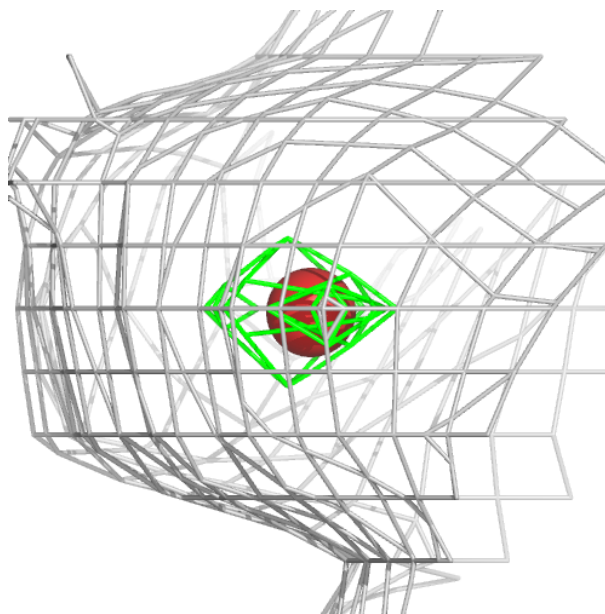
Electron density around BR B 502:

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and green (positive)



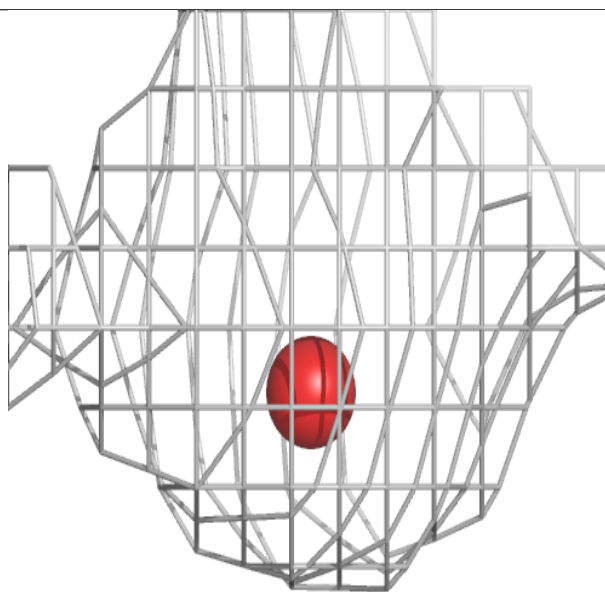
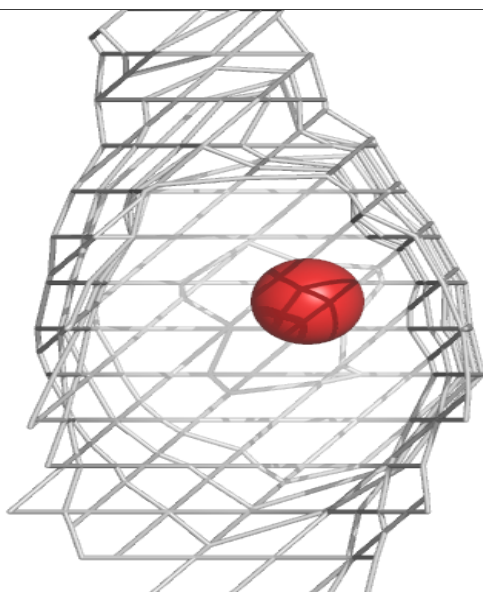
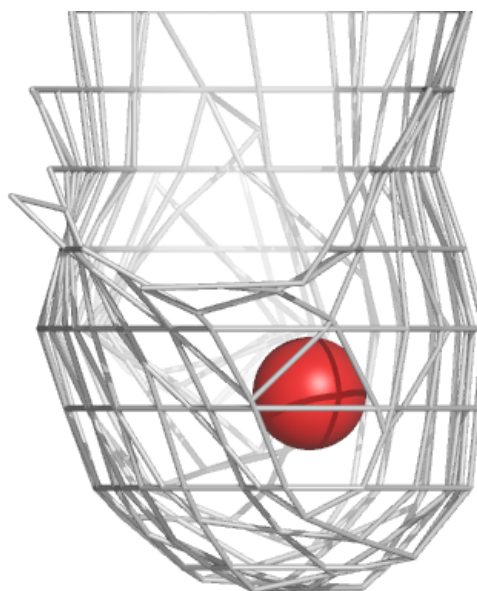
Electron density around BR A 501:

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



Electron density around BR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.