



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:37 PM UTC

PDB ID : 6ADB / pdb_00006adb
Title : Crystal structure of the E148N mutant CLC-ec1 in 20mM bromide
Authors : Lim, H.-H.; Park, K.
Deposited on : 2018-07-31
Resolution : 2.69 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

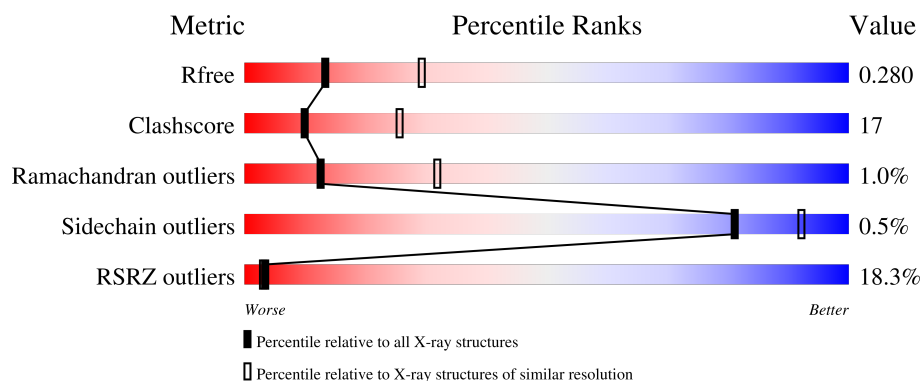
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	14% 65% 29% 6%
1	B	473	29% 61% 32% 7%
2	C	222	14% 74% 25% .
2	E	222	13% 75% 23% .
3	D	211	18% 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	BR	A	501	-	-	X	-
4	BR	A	502	-	-	X	-
4	BR	B	501	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13247 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	561	562	20			
1	B	442	Total	C	N	O	S	0	0	0
			3314	2179	558	557	20			

There are 2 discrepancies between the modelled and reference sequences:

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

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

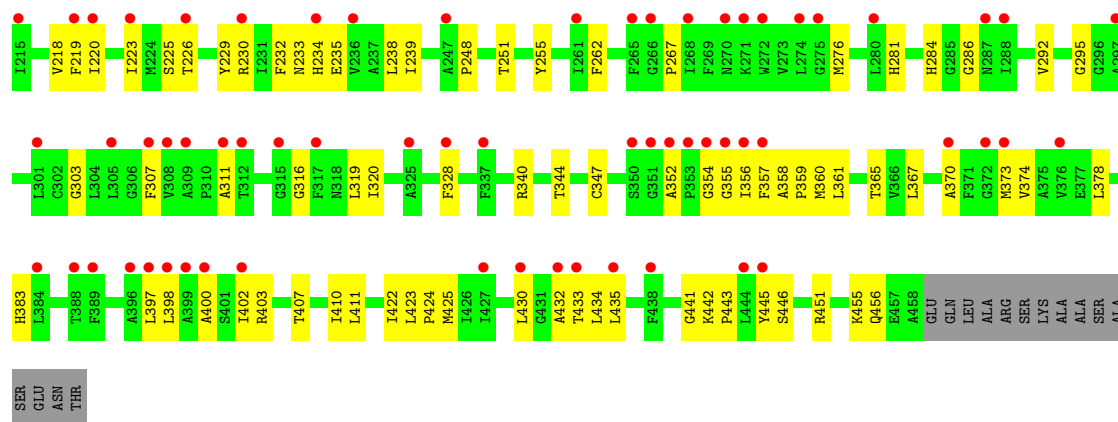
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1681	1082	275	318	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

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

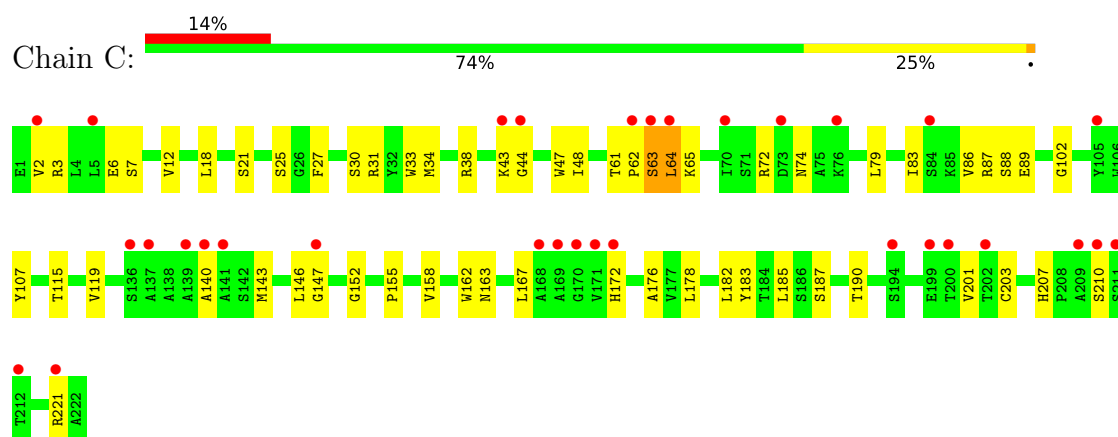
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

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

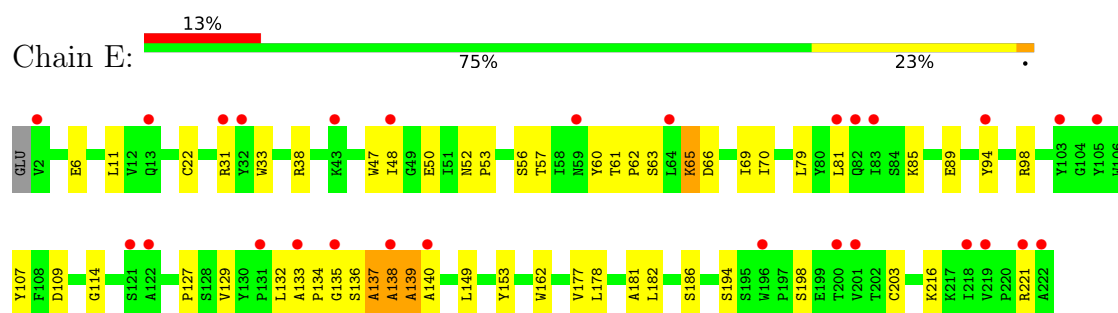
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Br 3	0	0
4	B	3	Total 3	Br 3	0	0



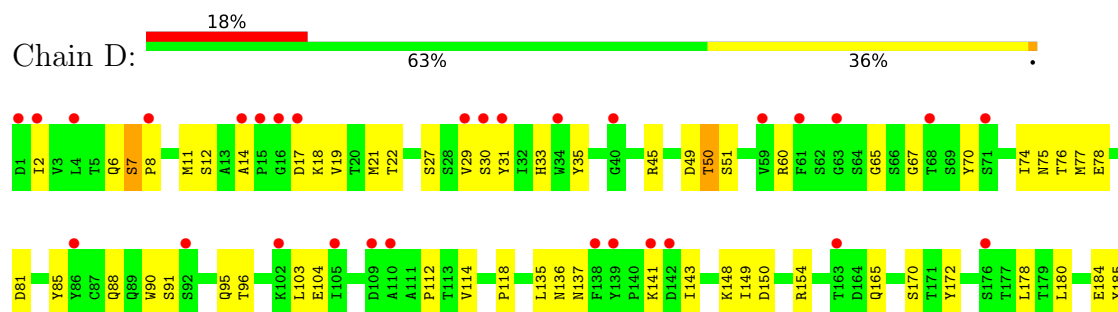
- Molecule 2: antibody Fab fragment, heavy chain

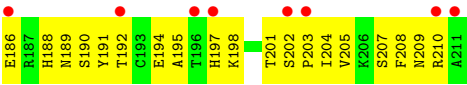


- Molecule 2: antibody Fab fragment, heavy chain



- 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	231.90Å 97.98Å 170.79Å 90.00° 132.02° 90.00°	Depositor
Resolution (Å)	33.96 – 2.69 33.96 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.96-2.69) 99.3 (33.96-2.69)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.237 , 0.278 0.242 , 0.280	Depositor DCC
R_{free} test set	3952 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13247	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: 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	0.47	1/3404 (0.0%)	0.63	0/4620
1	B	0.42	0/3386	0.69	2/4596 (0.0%)
2	C	0.46	0/1730	0.77	2/2367 (0.1%)
2	E	0.44	0/1721	0.67	0/2355
3	D	0.44	0/1660	0.76	0/2257
3	F	0.45	0/1660	0.70	0/2257
All	All	0.45	1/13561 (0.0%)	0.70	4/18452 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	PRO	N-CD	-13.96	1.28	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ARG	CA-C-N	-6.13	115.18	123.46
1	B	403	ARG	C-N-CA	-6.13	115.18	123.46
2	C	63	SER	CA-C-N	5.62	132.28	121.54
2	C	63	SER	C-N-CA	5.62	132.28	121.54

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	3332	0	3484	134	0
1	B	3314	0	3470	146	0
2	C	1681	0	1663	41	0
2	E	1672	0	1654	46	0
3	D	1621	0	1546	81	0
3	F	1621	0	1546	56	0
4	A	3	0	0	5	0
4	B	3	0	0	5	0
All	All	13247	0	13363	462	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 17.

All (462) 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	1.16	1.11
2:E:133:ALA:O	2:E:221:ARG:NH1	1.88	1.05
3:D:60:ARG:NH1	3:D:81:ASP:OD1	1.89	1.05
3:F:95:GLN:H	3:F:95:GLN:CD	1.66	1.03
3:D:95:GLN:OE1	3:D:95:GLN:N	1.94	1.00
3:D:6:GLN:NE2	3:D:85:TYR:O	1.98	0.96
3:F:95:GLN:N	3:F:95:GLN:OE1	1.99	0.94
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.00	0.90
1:A:146:GLY:HA3	4:A:501:BR:BR	2.27	0.89
1:B:18:ARG:H	1:B:18:ARG:HD3	1.36	0.89
1:B:320:ILE:HG23	1:B:365:THR:HG21	1.54	0.88
2:E:47:TRP:CD2	3:F:95:GLN:NE2	2.42	0.88
1:B:59:TRP:CE2	1:B:63:GLN:NE2	2.41	0.88
3:D:60:ARG:NH1	3:D:78:GLU:HB2	1.91	0.86
3:D:104:GLU:OE2	3:D:172:TYR:OH	1.95	0.84
3:F:192:THR:HG22	3:F:207:SER:HB3	1.60	0.84
1:A:98:ARG:HH22	1:A:102:PRO:HB3	1.44	0.82
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.63	0.81
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.63	0.81
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.16	0.80
3:D:60:ARG:HB2	3:D:74:ILE:CD1	2.11	0.80
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.62	0.80
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.63	0.80
2:E:134:PRO:C	2:E:221:ARG:NH1	2.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.64	0.79
2:E:134:PRO:C	2:E:221:ARG:HH11	1.90	0.78
3:D:60:ARG:HH12	3:D:78:GLU:HB2	1.50	0.77
2:E:70:ILE:HG13	2:E:81:LEU:HD12	1.68	0.76
1:A:18:ARG:NH2	1:B:456:GLN:CD	2.44	0.76
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.51	0.75
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.67	0.75
3:F:185:TYR:O	3:F:191:TYR:OH	2.05	0.75
1:A:176:THR:HG22	1:A:213:ILE:HA	1.67	0.75
1:A:126:ARG:O	1:A:130:VAL:HG12	1.87	0.75
2:E:135:GLY:O	2:E:137:ALA:N	2.20	0.75
1:A:430:LEU:HD11	1:B:219:PHE:CD1	2.22	0.74
3:F:194:GLU:HG2	3:F:205:VAL:HG13	1.69	0.74
3:D:31:TYR:HA	3:D:50:THR:HG23	1.70	0.74
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.68	0.74
2:C:30:SER:O	2:C:31:ARG:HB2	1.88	0.73
3:D:60:ARG:HD2	3:D:74:ILE:HD11	1.71	0.73
3:F:192:THR:HG22	3:F:207:SER:CB	2.18	0.73
1:A:207:GLN:NE2	1:B:28:ARG:HH11	1.86	0.73
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.71	0.73
2:E:89:GLU:N	2:E:89:GLU:OE2	2.22	0.72
1:B:145:LEU:HD11	1:B:347:CYS:HB3	1.72	0.72
1:B:72:ALA:HA	1:B:78:LEU:HD22	1.72	0.71
2:C:221:ARG:HH12	3:D:118:PRO:HD2	1.56	0.71
1:A:83:PHE:HD1	1:A:84:LEU:HD12	1.55	0.70
3:D:29:VAL:O	3:D:70:TYR:OH	2.07	0.70
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.73	0.70
1:B:229:TYR:OH	1:B:238:LEU:HD11	1.91	0.70
2:C:163:ASN:HD22	2:C:167:LEU:HD13	1.56	0.70
3:F:186:GLU:O	3:F:210:ARG:NH2	2.25	0.69
1:B:38:MET:HA	1:B:41:VAL:HG13	1.74	0.69
3:D:60:ARG:HB2	3:D:74:ILE:HD12	1.74	0.69
3:D:104:GLU:HB2	3:D:165:GLN:OE1	1.92	0.69
1:A:18:ARG:NH2	1:B:456:GLN:OE1	2.25	0.69
3:F:7:SER:HB3	3:F:22:THR:OG1	1.92	0.69
1:B:68:LEU:HD13	1:B:307:PHE:HD1	1.59	0.68
1:A:148:ASN:O	1:A:152:VAL:HG22	1.95	0.67
1:A:426:ILE:HG23	1:B:219:PHE:CE2	2.30	0.67
1:A:191:ASN:HD21	1:A:230:ARG:NH1	1.92	0.67
1:B:374:VAL:HG12	1:B:378:LEU:HD11	1.77	0.67
2:C:88:SER:HA	2:C:119:VAL:HG13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.10	0.66
3:D:60:ARG:HB2	3:D:74:ILE:HD11	1.76	0.66
1:B:182:ALA:HB1	1:B:204:MET:HE1	1.77	0.66
3:D:19:VAL:HB	3:D:74:ILE:CG2	2.25	0.66
3:F:192:THR:CG2	3:F:207:SER:HB3	2.26	0.66
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.77	0.66
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.78	0.65
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.61	0.65
1:B:239:ILE:HD11	1:B:320:ILE:CG2	2.26	0.65
2:E:47:TRP:CE3	3:F:95:GLN:NE2	2.64	0.65
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.28	0.65
1:A:210:TYR:HB3	1:B:209:ARG:HH11	1.61	0.65
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.03	0.65
3:D:154:ARG:HH12	3:D:180:LEU:HD21	1.62	0.65
3:D:192:THR:HG22	3:D:207:SER:HB2	1.79	0.65
2:E:134:PRO:O	2:E:221:ARG:NH1	2.31	0.64
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.12	0.64
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.80	0.64
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.79	0.64
1:A:376:VAL:HG12	1:A:384:LEU:HB2	1.79	0.64
2:C:64:LEU:HD12	2:C:65:LYS:H	1.61	0.64
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.80	0.64
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.80	0.64
1:B:20:GLN:O	1:B:24:GLN:HG3	1.98	0.64
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.81	0.63
1:B:20:GLN:OE1	1:B:24:GLN:NE2	2.32	0.63
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.34	0.62
2:E:149:LEU:HD12	2:E:186:SER:OG	2.00	0.62
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.82	0.62
2:C:207:HIS:HD2	2:C:210:SER:OG	1.83	0.62
1:B:17:ARG:O	1:B:20:GLN:HG3	2.00	0.62
1:B:59:TRP:CD2	1:B:63:GLN:NE2	2.62	0.61
1:A:255:TYR:CD1	1:A:424:PRO:HB3	2.36	0.61
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.82	0.61
1:A:271:LYS:NZ	1:A:275:GLY:HA3	2.16	0.61
1:A:422:ILE:HA	1:A:425:MET:HE3	1.81	0.61
2:E:85:LYS:HD2	2:E:85:LYS:N	2.15	0.61
1:A:447:ALA:O	1:A:451:ARG:HG3	2.00	0.61
1:B:112:ILE:HG23	1:B:178:LEU:HD21	1.83	0.61
2:C:87:ARG:HH11	2:C:89:GLU:HB3	1.66	0.61
1:B:360:MET:HE1	1:B:402:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:185:TYR:CZ	3:D:210:ARG:HD3	2.36	0.60
1:B:146:GLY:HA3	4:B:501:BR:BR	2.56	0.60
1:B:180:THR:HG22	1:B:218:VAL:HA	1.81	0.60
2:E:47:TRP:CE2	3:F:95:GLN:NE2	2.69	0.60
1:A:100:TYR:O	1:A:126:ARG:NH1	2.34	0.60
1:A:422:ILE:HD12	1:A:425:MET:HE3	1.82	0.60
1:B:219:PHE:O	1:B:223:ILE:HD12	2.01	0.60
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.37	0.60
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.02	0.60
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.37	0.59
3:D:75:ASN:O	3:D:76:THR:HG22	2.02	0.59
1:A:172:GLU:O	1:A:176:THR:HG23	2.02	0.59
2:C:2:VAL:HG23	2:C:27:PHE:CD1	2.37	0.59
3:F:180:LEU:HD22	3:F:184:GLU:HG2	1.83	0.59
1:A:276:MET:O	1:A:280:LEU:HD12	2.03	0.59
1:B:41:VAL:O	1:B:45:LEU:HG	2.03	0.59
2:C:7:SER:HA	2:C:115:THR:HG21	1.84	0.59
1:A:36:LEU:HD13	1:B:434:LEU:HD21	1.85	0.58
3:D:19:VAL:HG11	3:D:103:LEU:CD1	2.33	0.58
3:D:35:TYR:OH	3:D:88:GLN:OE1	2.15	0.58
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.84	0.58
3:D:7:SER:HB3	3:D:22:THR:HB	1.85	0.58
1:A:207:GLN:HE21	1:B:28:ARG:HD2	1.66	0.58
1:B:144:VAL:O	1:B:144:VAL:HG23	2.02	0.58
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.33	0.58
1:B:145:LEU:CD1	1:B:347:CYS:HB3	2.33	0.58
1:A:423:LEU:HD13	1:B:230:ARG:CZ	2.34	0.58
1:B:59:TRP:CZ2	1:B:63:GLN:NE2	2.71	0.58
1:B:234:HIS:CE1	1:B:235:GLU:HG3	2.39	0.58
3:D:19:VAL:HB	3:D:74:ILE:HG22	1.85	0.58
3:D:17:ASP:OD1	3:D:18:LYS:N	2.37	0.57
1:A:75:TYR:O	1:A:79:LEU:HD12	2.03	0.57
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.12	0.57
1:B:239:ILE:HD11	1:B:320:ILE:HG21	1.86	0.57
2:E:85:LYS:HD2	2:E:85:LYS:H	1.67	0.57
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.87	0.57
1:B:248:PRO:O	1:B:251:THR:HB	2.05	0.57
1:A:146:GLY:CA	4:A:501:BR:BR	3.06	0.57
1:B:66:GLY:O	1:B:69:VAL:HG12	2.04	0.57
2:C:12:VAL:HG11	2:C:18:LEU:HD23	1.86	0.57
1:A:176:THR:HG22	1:A:214:SER:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:HA	1:B:361:LEU:HD12	1.86	0.57
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.40	0.57
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.39	0.57
1:A:207:GLN:HE21	1:B:28:ARG:HH11	1.48	0.57
1:B:38:MET:O	1:B:42:VAL:HG23	2.05	0.57
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.87	0.57
2:E:133:ALA:C	2:E:221:ARG:HH12	2.05	0.57
1:A:276:MET:HG3	1:A:280:LEU:CD1	2.34	0.56
2:E:47:TRP:CG	3:F:95:GLN:HE21	2.19	0.56
1:A:346:LEU:O	1:A:350:SER:HB3	2.05	0.56
1:B:267:PRO:HB3	1:B:441:GLY:HA3	1.86	0.56
1:B:110:PRO:HG2	4:B:503:BR:BR	2.61	0.56
1:B:68:LEU:HA	1:B:78:LEU:HD11	1.88	0.56
1:A:92:PHE:O	1:A:96:LEU:HD12	2.06	0.56
1:A:138:THR:HG21	1:A:353:PRO:O	2.06	0.56
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.71	0.56
1:A:271:LYS:HZ3	1:A:275:GLY:HA3	1.71	0.55
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.88	0.55
1:A:191:ASN:ND2	1:A:230:ARG:NH1	2.54	0.55
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.70	0.55
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.89	0.55
1:A:381:GLN:OE1	1:A:381:GLN:N	2.27	0.55
1:B:176:THR:O	1:B:180:THR:HG23	2.07	0.55
1:B:402:ILE:HD12	1:B:402:ILE:N	2.22	0.55
3:F:145:VAL:HG11	3:F:174:MET:HE1	1.89	0.55
3:F:148:LYS:HA	3:F:152:SER:O	2.08	0.54
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.88	0.54
3:F:144:ASN:HB2	3:F:196:THR:OG1	2.06	0.54
1:A:92:PHE:CZ	1:A:96:LEU:HD11	2.43	0.54
3:F:38:LYS:O	3:F:41:THR:HB	2.07	0.54
1:B:145:LEU:HD23	1:B:354:GLY:C	2.32	0.54
1:A:77:LEU:O	1:A:81:VAL:HG23	2.07	0.54
3:F:186:GLU:C	3:F:188:HIS:H	2.16	0.54
1:B:132:PHE:O	1:B:136:LEU:HG	2.08	0.54
2:E:149:LEU:HD13	3:F:132:VAL:HG21	1.89	0.54
3:F:192:THR:CB	3:F:207:SER:HB3	2.38	0.54
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.43	0.53
3:F:182:LYS:O	3:F:186:GLU:HG3	2.08	0.53
1:A:176:THR:CG2	1:A:214:SER:H	2.21	0.53
3:F:181:THR:HG23	3:F:184:GLU:H	1.73	0.53
2:C:43:LYS:CD	2:C:44:GLY:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:145:VAL:HA	3:F:194:GLU:O	2.08	0.53
1:B:47:GLY:O	1:B:51:VAL:HG23	2.08	0.53
3:F:95:GLN:CD	3:F:95:GLN:N	2.45	0.53
1:B:255:TYR:CD1	1:B:424:PRO:HB3	2.44	0.53
3:D:60:ARG:NH1	3:D:78:GLU:CB	2.69	0.53
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.90	0.53
1:A:355:GLY:HA3	4:A:501:BR:BR	2.64	0.52
1:B:109:ILE:HB	1:B:110:PRO:HD3	1.91	0.52
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.44	0.52
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.44	0.52
1:A:220:ILE:HD11	1:B:434:LEU:HD11	1.92	0.52
3:F:44:LYS:NZ	3:F:54:THR:HG21	2.25	0.52
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.43	0.52
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.73	0.52
2:C:43:LYS:HD2	2:C:44:GLY:H	1.74	0.52
1:A:191:ASN:HD21	1:A:230:ARG:HH11	1.57	0.52
2:C:143:MET:HE3	2:C:190:THR:HG22	1.91	0.52
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.42	0.52
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.45	0.52
3:D:60:ARG:CD	3:D:74:ILE:HD11	2.40	0.52
1:A:94:TYR:CE1	1:A:295:GLY:HA3	2.45	0.52
2:C:87:ARG:O	2:C:119:VAL:HG11	2.10	0.52
3:F:30:SER:HA	3:F:70:TYR:OH	2.10	0.52
3:D:14:ALA:O	3:D:17:ASP:HB3	2.10	0.51
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.93	0.51
2:C:152:GLY:HA2	2:C:182:LEU:HB3	1.91	0.51
2:C:162:TRP:CH2	2:C:203:CYS:HB3	2.45	0.51
1:B:144:VAL:CG2	1:B:344:THR:HA	2.40	0.51
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.93	0.51
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.10	0.51
1:B:148:ASN:HB3	4:B:501:BR:BR	2.65	0.51
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.46	0.51
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.92	0.51
3:D:180:LEU:HD23	3:D:184:GLU:OE1	2.09	0.51
1:B:451:ARG:O	1:B:455:LYS:HE2	2.11	0.51
1:B:422:ILE:HA	1:B:425:MET:HE3	1.93	0.51
2:C:12:VAL:O	2:C:119:VAL:HA	2.12	0.50
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.11	0.50
3:D:197:HIS:CG	3:D:198:LYS:H	2.29	0.50
1:A:191:ASN:ND2	1:A:230:ARG:HH11	2.10	0.50
1:B:144:VAL:HG21	1:B:344:THR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.80	0.50
1:B:20:GLN:HA	1:B:23:ARG:NH1	2.27	0.50
2:E:47:TRP:HZ2	2:E:50:GLU:HG2	1.77	0.50
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.93	0.49
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.93	0.49
3:D:31:TYR:HA	3:D:50:THR:CG2	2.39	0.49
2:E:38:ARG:HD3	2:E:48:ILE:HD11	1.94	0.49
2:E:137:ALA:O	2:E:139:ALA:N	2.42	0.49
1:A:180:THR:HB	1:A:218:VAL:HA	1.93	0.49
2:C:155:PRO:O	2:C:207:HIS:HE1	1.95	0.49
3:D:136:ASN:HB3	3:D:137:ASN:HD22	1.78	0.49
1:B:148:ASN:HD21	1:B:186:LEU:HD12	1.77	0.49
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.95	0.49
1:B:77:LEU:O	1:B:81:VAL:HG12	2.13	0.49
1:B:61:GLN:OE1	1:B:64:ARG:NH2	2.46	0.49
3:D:191:TYR:HB2	3:D:208:PHE:CE2	2.47	0.49
1:A:109:ILE:HG12	1:A:152:VAL:HG21	1.94	0.49
1:B:284:HIS:C	1:B:286:GLY:H	2.21	0.49
3:F:80:GLU:HA	3:F:167:SER:O	2.13	0.49
1:B:200:ILE:CD1	1:B:204:MET:HE2	2.42	0.49
1:A:83:PHE:CD1	1:A:84:LEU:HD12	2.42	0.49
1:A:18:ARG:NH2	1:B:456:GLN:NE2	2.61	0.48
1:A:88:VAL:HA	1:A:91:MET:HE2	1.95	0.48
1:A:270:ASN:ND2	1:A:444:LEU:HD13	2.28	0.48
1:A:69:VAL:C	1:A:71:THR:H	2.21	0.48
1:A:144:VAL:O	1:A:145:LEU:HG	2.14	0.48
3:D:74:ILE:HG12	3:D:81:ASP:OD2	2.12	0.48
2:C:172:HIS:HE1	3:D:136:ASN:CG	2.21	0.48
1:A:186:LEU:HD22	1:A:196:GLY:HA2	1.96	0.48
3:D:30:SER:H	3:D:91:SER:HB3	1.78	0.48
2:E:6:GLU:CD	2:E:114:GLY:H	2.20	0.48
3:F:20:THR:HG23	3:F:73:THR:OG1	2.13	0.48
2:E:177:VAL:HG11	3:F:159:LEU:HD13	1.95	0.48
1:A:97:VAL:HA	1:A:130:VAL:HG21	1.95	0.48
1:B:360:MET:HE1	1:B:402:ILE:CD1	2.44	0.48
1:B:355:GLY:HA3	4:B:501:BR:BR	2.69	0.48
3:D:186:GLU:O	3:D:210:ARG:NH2	2.47	0.48
1:A:152:VAL:HG12	1:A:182:ALA:O	2.14	0.48
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.95	0.48
2:E:133:ALA:C	2:E:221:ARG:NH1	2.67	0.48
1:A:188:ALA:HB2	1:A:225:SER:OG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASN:CG	1:A:230:ARG:HH11	2.22	0.47
1:A:226:THR:HG21	1:B:423:LEU:HD11	1.95	0.47
2:C:86:VAL:HG12	2:C:119:VAL:HG21	1.96	0.47
3:D:60:ARG:C	3:D:74:ILE:HD12	2.39	0.47
3:D:7:SER:CB	3:D:8:PRO:HD3	2.43	0.47
3:F:66:SER:HA	3:F:70:TYR:CZ	2.48	0.47
3:F:154:ARG:HE	3:F:156:ASN:HB2	1.79	0.47
1:A:25:LEU:HD23	1:B:208:PHE:HE1	1.79	0.47
2:C:107:TYR:HB3	3:D:33:HIS:CE1	2.49	0.47
2:E:132:LEU:HD11	2:E:149:LEU:HB2	1.95	0.47
3:F:150:ASP:HA	3:F:190:SER:HB3	1.97	0.47
1:B:328:PHE:O	1:B:373:MET:HE1	2.14	0.47
1:B:441:GLY:C	1:B:442:LYS:HG3	2.39	0.47
3:D:2:ILE:O	3:D:96:THR:HG21	2.14	0.47
1:B:71:THR:HB	1:B:77:LEU:HD23	1.95	0.47
3:D:77:MET:HE1	3:D:103:LEU:HD11	1.97	0.47
2:E:66:ASP:HB3	2:E:69:ILE:HD11	1.96	0.47
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.49	0.47
1:A:109:ILE:HG23	1:A:204:MET:SD	2.55	0.47
1:B:51:VAL:HG11	1:B:232:PHE:HB2	1.97	0.47
1:A:148:ASN:HD21	1:A:186:LEU:HD12	1.80	0.47
3:D:104:GLU:OE1	3:D:141:LYS:HE2	2.15	0.47
2:E:70:ILE:CG1	2:E:81:LEU:HD12	2.43	0.47
1:A:251:THR:HG22	1:A:255:TYR:CE1	2.49	0.46
1:A:399:ALA:O	1:A:403:ARG:HA	2.16	0.46
1:A:411:LEU:HG	1:A:415:MET:HE2	1.98	0.46
1:B:68:LEU:HD13	1:B:307:PHE:CD1	2.44	0.46
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.72	0.46
1:B:430:LEU:HA	1:B:433:THR:HG22	1.98	0.46
2:C:18:LEU:HD11	2:C:83:ILE:HD12	1.97	0.46
3:D:112:PRO:HG3	3:D:143:ILE:HD11	1.96	0.46
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.64	0.46
1:B:53:PHE:O	1:B:57:VAL:HG23	2.16	0.46
2:C:87:ARG:HH11	2:C:89:GLU:CB	2.28	0.46
1:B:91:MET:HG2	1:B:292:VAL:O	2.14	0.46
3:D:60:ARG:NH1	3:D:78:GLU:HG2	2.31	0.46
1:A:422:ILE:HA	1:A:422:ILE:HD12	1.79	0.46
1:B:118:ASP:OD1	1:B:174:ARG:NH2	2.29	0.46
1:B:360:MET:HE3	1:B:360:MET:HB2	1.61	0.46
1:B:374:VAL:HG12	1:B:378:LEU:CD1	2.45	0.46
1:A:91:MET:HG2	1:A:292:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:HB1	1:A:204:MET:HE1	1.97	0.46
1:B:445:TYR:OH	4:B:502:BR:BR	2.77	0.46
1:B:229:TYR:O	1:B:233:ASN:HB2	2.16	0.46
1:B:360:MET:SD	1:B:402:ILE:HD11	2.56	0.46
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.51	0.46
1:A:160:ARG:NE	1:A:163:LEU:HD23	2.31	0.45
3:F:49:ASP:O	3:F:50:THR:HB	2.17	0.45
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.68	0.45
1:B:116:LEU:HG	1:B:178:LEU:HD22	1.98	0.45
3:D:198:LYS:HD2	3:D:198:LYS:HA	1.86	0.45
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.71	0.45
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.97	0.45
1:B:120:ARG:HE	1:B:120:ARG:HB3	1.42	0.45
1:B:199:PHE:CD1	1:B:407:THR:HG21	2.52	0.45
1:A:53:PHE:O	1:A:57:VAL:HG23	2.16	0.45
1:A:223:ILE:HD11	1:B:430:LEU:HD22	1.98	0.45
1:A:276:MET:HG3	1:A:280:LEU:HD12	1.99	0.45
2:C:61:THR:O	2:C:63:SER:N	2.49	0.45
3:D:76:THR:O	3:D:76:THR:HG23	2.17	0.45
3:D:149:ILE:HD11	3:D:178:LEU:HD21	1.99	0.45
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.98	0.45
1:B:78:LEU:HD12	1:B:78:LEU:HA	1.55	0.45
1:B:19:ARG:O	1:B:23:ARG:HG2	2.17	0.45
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.65	0.45
2:E:194:SER:O	2:E:198:SER:HB3	2.16	0.45
1:A:51:VAL:O	1:A:55:LYS:HG2	2.17	0.45
1:B:206:PRO:CG	1:B:211:THR:HG21	2.45	0.45
1:A:226:THR:CG2	1:B:423:LEU:HD11	2.47	0.44
1:B:356:ILE:C	1:B:359:PRO:HD2	2.42	0.44
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.53	0.44
1:A:361:LEU:HD13	1:A:415:MET:HE1	2.00	0.44
1:A:120:ARG:HE	1:A:120:ARG:HB3	1.56	0.44
1:A:219:PHE:CG	1:B:430:LEU:HD11	2.52	0.44
1:B:75:TYR:O	1:B:79:LEU:HG	2.17	0.44
3:D:150:ASP:HA	3:D:190:SER:OG	2.17	0.44
2:E:129:VAL:O	2:E:216:LYS:HE3	2.17	0.44
3:F:196:THR:HG22	3:F:203:PRO:HB3	1.99	0.44
3:D:35:TYR:CD2	3:D:45:ARG:HA	2.52	0.44
1:A:373:MET:HA	1:A:376:VAL:HG22	2.00	0.44
1:A:430:LEU:CD2	1:B:223:ILE:HD11	2.48	0.44
1:B:86:SER:OG	1:B:303:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.88	0.44
2:E:60:TYR:CE2	2:E:70:ILE:HD12	2.52	0.44
1:A:86:SER:OG	1:A:303:GLY:HA3	2.17	0.44
2:C:3:ARG:HB2	2:C:25:SER:OG	2.17	0.44
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.17	0.44
3:F:112:PRO:HG3	3:F:143:ILE:HD11	1.99	0.44
3:D:194:GLU:HG2	3:D:205:VAL:CG1	2.11	0.44
2:E:11:LEU:HD12	2:E:11:LEU:HA	1.81	0.44
1:A:144:VAL:C	1:A:145:LEU:HG	2.43	0.43
1:A:276:MET:HG3	1:A:280:LEU:HD11	2.00	0.43
3:D:19:VAL:HG11	3:D:103:LEU:HD13	1.99	0.43
1:B:42:VAL:O	1:B:46:VAL:HG23	2.18	0.43
1:A:265:PHE:CD2	1:A:397:LEU:HD21	2.53	0.43
1:B:94:TYR:CE1	1:B:295:GLY:HA3	2.54	0.43
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.35	0.43
3:D:30:SER:HB3	3:D:31:TYR:CD2	2.52	0.43
3:D:49:ASP:O	3:D:51:SER:N	2.50	0.43
1:A:320:ILE:HD13	1:A:394:MET:HE3	1.99	0.43
1:A:423:LEU:HD11	1:B:226:THR:HG21	1.99	0.43
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.99	0.43
3:D:74:ILE:HG21	3:D:77:MET:HE3	2.00	0.43
3:D:77:MET:HE1	3:D:103:LEU:CD1	2.49	0.43
1:A:376:VAL:HG12	1:A:384:LEU:CB	2.48	0.43
2:C:158:VAL:HG12	2:C:207:HIS:HB2	2.00	0.43
3:D:165:GLN:HE21	3:D:170:SER:HB3	1.84	0.43
1:B:238:LEU:N	1:B:238:LEU:HD12	2.33	0.43
2:C:6:GLU:HA	2:C:21:SER:O	2.18	0.43
1:A:210:TYR:HB2	1:B:209:ARG:HD2	2.00	0.43
3:F:44:LYS:HZ1	3:F:54:THR:HG21	1.83	0.43
1:A:81:VAL:O	1:A:85:CYS:HB2	2.19	0.43
1:B:370:ALA:O	1:B:374:VAL:HG23	2.18	0.42
2:C:221:ARG:HH12	3:D:118:PRO:CD	2.29	0.42
3:D:30:SER:H	3:D:91:SER:CB	2.31	0.42
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.87	0.42
3:D:165:GLN:NE2	3:D:170:SER:HB3	2.34	0.42
1:B:98:ARG:HH21	1:B:102:PRO:HB3	1.83	0.42
1:B:234:HIS:CE1	2:C:102:GLY:O	2.72	0.42
1:A:294:MET:HE2	1:A:294:MET:HB3	1.97	0.42
1:A:445:TYR:OH	4:A:502:BR:BR	2.84	0.42
3:F:60:ARG:HG3	3:F:74:ILE:HG23	2.01	0.42
3:F:149:ILE:HG12	3:F:191:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ALA:HB1	1:B:225:SER:CB	2.47	0.42
1:B:383:HIS:CE1	3:F:90:TRP:CZ2	3.07	0.42
2:C:38:ARG:CD	2:C:48:ILE:HD11	2.49	0.42
3:D:60:ARG:NH1	3:D:78:GLU:CG	2.83	0.42
2:E:138:ALA:O	2:E:140:ALA:N	2.51	0.42
1:A:18:ARG:HH22	1:B:456:GLN:NE2	2.18	0.42
1:A:234:HIS:O	1:A:235:GLU:HB2	2.19	0.42
2:E:94:TYR:O	2:E:114:GLY:HA2	2.20	0.42
1:A:248:PRO:O	1:A:251:THR:HB	2.20	0.42
1:A:397:LEU:O	1:A:401:SER:HB2	2.19	0.42
1:B:200:ILE:HD12	1:B:204:MET:HE2	2.01	0.42
1:B:311:ALA:O	1:B:340:ARG:HD2	2.19	0.42
1:B:360:MET:CE	1:B:402:ILE:HD11	2.49	0.42
3:D:192:THR:HG22	3:D:207:SER:CB	2.49	0.42
1:A:119:GLN:C	1:A:120:ARG:HG2	2.44	0.42
1:A:219:PHE:O	1:A:223:ILE:HG13	2.20	0.42
1:B:38:MET:HE3	1:B:38:MET:HB3	1.74	0.42
3:D:12:SER:HA	3:D:104:GLU:O	2.19	0.42
2:E:52:ASN:HD21	2:E:56:SER:HB3	1.84	0.42
3:D:11:MET:HE1	3:D:21:MET:HB3	2.02	0.42
3:D:202:SER:HA	3:D:203:PRO:HD2	1.94	0.42
3:F:159:LEU:HA	3:F:159:LEU:HD23	1.77	0.42
1:B:138:THR:HG23	1:B:143:MET:HE3	2.02	0.41
3:D:150:ASP:OD1	3:D:188:HIS:HB3	2.20	0.41
3:D:195:ALA:HB3	3:D:204:ILE:HG23	2.02	0.41
3:F:7:SER:OG	3:F:8:PRO:CD	2.68	0.41
1:A:69:VAL:C	1:A:71:THR:N	2.77	0.41
1:A:309:ALA:O	1:A:312:THR:OG1	2.32	0.41
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.38	0.41
1:B:78:LEU:HA	1:B:81:VAL:HG12	2.02	0.41
2:C:147:GLY:HA2	2:C:187:SER:O	2.20	0.41
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.35	0.41
2:E:61:THR:O	2:E:63:SER:N	2.53	0.41
1:A:357:PHE:HB2	4:A:502:BR:BR	2.76	0.41
2:E:52:ASN:CG	2:E:57:THR:H	2.27	0.41
1:A:75:TYR:CZ	1:A:79:LEU:HD11	2.55	0.41
1:A:403:ARG:NH2	1:B:29:ASP:OD2	2.46	0.41
1:B:68:LEU:HD21	1:B:82:ALA:HB2	2.01	0.41
3:D:189:ASN:O	3:D:209:ASN:HA	2.21	0.41
3:F:196:THR:CG2	3:F:203:PRO:HB3	2.51	0.41
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.02	0.41
1:A:94:TYR:OH	1:A:352:ALA:HB2	2.21	0.41
1:A:182:ALA:CB	1:A:204:MET:HE1	2.51	0.41
1:B:316:GLY:O	1:B:319:LEU:HG	2.20	0.41
1:B:360:MET:HE3	1:B:398:LEU:HD23	2.02	0.41
2:E:178:LEU:HD11	2:E:181:ALA:HA	2.02	0.41
3:F:7:SER:HB2	3:F:8:PRO:HD3	2.03	0.41
3:F:184:GLU:HA	3:F:187:ARG:HG2	2.03	0.41
3:F:189:ASN:ND2	3:F:209:ASN:OD1	2.54	0.41
1:A:130:VAL:O	1:A:134:GLY:N	2.46	0.41
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.55	0.41
1:B:103:GLU:O	1:B:111:GLU:HG3	2.21	0.41
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.56	0.41
2:E:133:ALA:O	2:E:221:ARG:CZ	2.63	0.41
2:E:178:LEU:HD12	2:E:182:LEU:O	2.21	0.41
1:A:118:ASP:OD2	1:A:174:ARG:NH2	2.53	0.41
1:B:358:ALA:O	1:B:361:LEU:HB2	2.20	0.41
3:D:194:GLU:CD	3:D:205:VAL:HG12	2.45	0.41
3:F:116:ILE:HD12	3:F:193:CYS:SG	2.61	0.41
1:B:422:ILE:HA	1:B:425:MET:CE	2.51	0.40
3:D:19:VAL:HG21	3:D:77:MET:SD	2.61	0.40
2:E:65:LYS:CD	2:E:65:LYS:H	2.35	0.40
1:A:272:TRP:N	1:A:272:TRP:CD1	2.89	0.40
1:A:320:ILE:HB	1:A:321:PRO:HD3	2.02	0.40
1:B:435:LEU:HD13	1:B:435:LEU:HA	1.90	0.40
2:E:31:ARG:H	2:E:53:PRO:HB3	1.85	0.40
3:F:77:MET:HB3	3:F:77:MET:HE2	1.49	0.40
1:B:239:ILE:HD11	1:B:320:ILE:CB	2.50	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%)	417 (94%)	23 (5%)	2 (0%)	24	48
1	B	440/473 (93%)	418 (95%)	20 (4%)	2 (0%)	24	48
2	C	220/222 (99%)	203 (92%)	14 (6%)	3 (1%)	9	23
2	E	219/222 (99%)	201 (92%)	12 (6%)	6 (3%)	4	10
3	D	209/211 (99%)	193 (92%)	13 (6%)	3 (1%)	9	23
3	F	209/211 (99%)	198 (95%)	9 (4%)	2 (1%)	12	32
All	All	1739/1812 (96%)	1630 (94%)	91 (5%)	18 (1%)	12	32

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
3	D	50	THR
2	E	65	LYS
2	E	136	SER
3	F	7	SER
1	B	210	TYR
3	D	67	GLY
2	E	138	ALA
1	A	457	GLU
2	E	139	ALA
1	B	29	ASP
2	C	62	PRO
2	C	140	ALA
3	D	7	SER
2	E	137	ALA
2	E	62	PRO
3	F	76	THR
1	A	213	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/358 (94%)	332 (99%)	3 (1%)	70	87
1	B	333/358 (93%)	331 (99%)	2 (1%)	78	91
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%)	184 (100%)	1 (0%)	81	92
3	F	185/185 (100%)	184 (100%)	1 (0%)	81	92
All	All	1401/1450 (97%)	1394 (100%)	7 (0%)	81	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	180	THR
1	A	276	MET
1	B	41	VAL
1	B	276	MET
3	D	201	THR
3	F	95	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	157	ASN
1	A	175	HIS
1	A	207	GLN
1	A	270	ASN
1	A	281	HIS
1	B	24	GLN
1	B	157	ASN
1	B	234	HIS
1	B	270	ASN
1	B	284	HIS
2	C	163	ASN
2	C	172	HIS
2	C	207	HIS
3	D	37	GLN

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Mol	Chain	Res	Type
3	D	136	ASN
3	D	137	ASN
2	E	172	HIS
3	F	36	GLN
3	F	75	ASN
3	F	137	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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%)	1.02	66 (14%) 5 4	62, 88, 119, 166	0
1	B	442/473 (93%)	1.57	136 (30%) 1 1	65, 91, 134, 173	0
2	C	222/222 (100%)	0.96	32 (14%) 6 5	53, 80, 125, 179	0
2	E	221/222 (99%)	0.85	28 (12%) 8 7	55, 80, 120, 165	0
3	D	211/211 (100%)	1.23	38 (18%) 3 3	61, 91, 111, 132	0
3	F	211/211 (100%)	0.83	21 (9%) 12 10	54, 74, 117, 148	0
All	All	1751/1812 (96%)	1.13	321 (18%) 3 3	53, 86, 122, 179	0

All (321) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	ALA	9.1
1	B	354	GLY	6.7
1	B	159	GLY	6.3
1	B	215	ILE	6.3
1	A	283	VAL	6.3
1	B	104	ALA	6.3
1	B	223	ILE	6.1
1	A	440	GLY	6.0
1	B	139	LEU	6.0
2	E	201	VAL	5.9
3	D	211	ALA	5.4
1	B	353	PRO	5.2
1	A	219	PHE	5.2
1	A	392	ALA	5.1
3	F	158	VAL	5.0
3	D	110	ALA	4.8
1	B	210	TYR	4.8
3	D	16	GLY	4.8
1	B	33	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	355	GLY	4.7
1	B	95	PHE	4.7
1	B	270	ASN	4.7
1	A	29	ASP	4.6
3	F	169	ASP	4.6
1	B	162	VAL	4.6
2	C	147	GLY	4.5
2	C	141	ALA	4.5
1	A	171	ASP	4.4
2	E	103	TYR	4.4
1	B	177	LEU	4.4
1	B	213	ILE	4.4
1	B	127	VAL	4.4
1	A	393	GLY	4.3
1	B	266	GLY	4.2
1	B	271	LYS	4.2
2	C	64	LEU	4.1
2	E	121	SER	4.1
2	E	81	LEU	4.1
1	B	89	LEU	4.0
1	B	397	LEU	4.0
1	B	226	THR	3.9
1	B	36	LEU	3.9
1	B	430	LEU	3.9
1	B	201	ILE	3.8
1	A	77	LEU	3.8
2	C	140	ALA	3.8
1	B	200	ILE	3.8
1	B	168	LEU	3.7
1	B	399	ALA	3.7
2	C	169	ALA	3.7
2	E	13	GLN	3.7
2	E	221	ARG	3.7
3	D	142	ASP	3.7
1	A	262	PHE	3.7
1	A	439	THR	3.6
3	D	192	THR	3.6
2	E	59	ASN	3.6
2	E	133	ALA	3.6
1	B	148	ASN	3.6
2	C	199	GLU	3.5
1	B	351	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	200	THR	3.4
1	B	372	GLY	3.4
1	B	178	LEU	3.4
1	A	275	GLY	3.4
1	B	21	LEU	3.4
1	B	145	LEU	3.4
3	F	7	SER	3.3
1	A	25	LEU	3.3
1	B	116	LEU	3.3
1	B	352	ALA	3.3
1	B	402	ILE	3.3
3	D	86	TYR	3.3
2	E	135	GLY	3.3
2	E	122	ALA	3.3
1	B	208	PHE	3.3
1	B	376	VAL	3.3
3	F	205	VAL	3.3
1	B	125	TRP	3.2
1	B	317	PHE	3.2
2	E	31	ARG	3.2
3	F	156	ASN	3.1
1	A	145	LEU	3.1
1	A	212	LEU	3.1
1	B	22	ILE	3.1
1	B	166	PHE	3.1
1	A	147	ARG	3.1
1	B	115	ALA	3.1
1	B	311	ALA	3.1
1	A	143	MET	3.1
1	B	92	PHE	3.1
1	B	204	MET	3.1
3	D	139	TYR	3.0
1	B	80	THR	3.0
1	B	275	GLY	3.0
1	A	339	ALA	3.0
1	B	309	ALA	3.0
1	B	388	THR	3.0
3	D	196	THR	3.0
3	D	2	ILE	3.0
1	A	67	ALA	3.0
1	B	398	LEU	3.0
1	B	157	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	8	PRO	2.9
3	D	1	ASP	2.9
2	C	168	ALA	2.9
3	D	14	ALA	2.9
1	A	125	TRP	2.9
2	E	94	TYR	2.9
1	B	288	ILE	2.9
1	A	428	THR	2.9
1	B	325	ALA	2.9
1	B	83	PHE	2.9
2	C	136	SER	2.9
3	F	149	ILE	2.9
2	C	210	SER	2.9
1	B	315	GLY	2.9
3	F	151	GLY	2.9
1	A	341	VAL	2.9
3	D	61	PHE	2.9
1	B	18	ARG	2.8
3	D	138	PHE	2.8
1	A	213	ILE	2.8
1	B	268	ILE	2.8
1	B	350	SER	2.8
3	D	105	ILE	2.8
1	B	274	LEU	2.8
1	B	384	LEU	2.8
1	B	72	ALA	2.8
1	A	235	GLU	2.8
1	B	23	ARG	2.8
2	C	76	LYS	2.8
2	E	218	ILE	2.8
3	D	63	GLY	2.8
2	C	202	THR	2.8
1	A	448	ILE	2.8
1	A	58	ALA	2.8
3	F	168	LYS	2.7
2	E	83	ILE	2.7
3	F	204	ILE	2.7
3	D	202	SER	2.7
3	F	200	SER	2.7
1	A	438	PHE	2.7
1	B	94	TYR	2.7
3	D	31	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	373	MET	2.7
1	B	301	LEU	2.7
3	F	157	GLY	2.7
3	D	29	VAL	2.7
3	F	193	CYS	2.7
2	C	170	GLY	2.7
1	B	370	ALA	2.7
2	E	2	VAL	2.7
2	E	138	ALA	2.7
2	E	48	ILE	2.6
1	B	163	LEU	2.6
1	A	169	LYS	2.6
2	E	140	ALA	2.6
3	D	59	VAL	2.6
3	D	203	PRO	2.6
3	F	31	TYR	2.6
1	B	308	VAL	2.6
2	C	63	SER	2.6
2	C	171	VAL	2.6
2	E	131	PRO	2.6
3	F	22	THR	2.6
3	F	147	TRP	2.6
1	B	35	ILE	2.6
1	B	143	MET	2.6
3	D	4	LEU	2.6
1	A	234	HIS	2.6
1	B	328	PHE	2.6
1	B	389	PHE	2.6
3	D	15	PRO	2.6
3	D	30	SER	2.6
1	B	112	ILE	2.6
1	B	212	LEU	2.6
1	A	122	VAL	2.6
1	A	447	ALA	2.6
1	B	179	ALA	2.6
1	B	206	PRO	2.6
1	B	219	PHE	2.6
1	B	396	ALA	2.6
1	B	209	ARG	2.5
2	C	221	ARG	2.5
1	B	444	LEU	2.5
1	B	93	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	183	ALA	2.5
2	E	82	GLN	2.5
1	B	65	MET	2.5
1	B	427	ILE	2.5
2	C	139	ALA	2.5
3	D	141	LYS	2.5
1	B	220	ILE	2.5
2	C	62	PRO	2.5
1	B	57	VAL	2.5
3	F	155	GLN	2.5
1	B	305	LEU	2.4
3	D	34	TRP	2.4
1	B	337	PHE	2.4
1	B	438	PHE	2.4
1	A	21	LEU	2.4
2	E	64	LEU	2.4
2	C	194	SER	2.4
1	B	66	GLY	2.4
1	A	342	ILE	2.4
1	B	138	THR	2.4
1	B	280	LEU	2.4
3	D	109	ASP	2.4
1	B	38	MET	2.4
1	A	207	GLN	2.4
1	A	279	LEU	2.4
1	B	435	LEU	2.4
3	F	144	ASN	2.4
3	D	186	GLU	2.4
1	B	307	PHE	2.4
2	C	209	ALA	2.4
1	A	139	LEU	2.3
2	E	105	TYR	2.3
1	B	234	HIS	2.3
3	D	17	ASP	2.3
1	B	121	PRO	2.3
1	B	126	ARG	2.3
1	B	180	THR	2.3
1	B	433	THR	2.3
3	F	196	THR	2.3
1	A	170	GLY	2.3
1	B	247	ALA	2.3
2	C	137	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	356	ILE	2.3
1	A	407	THR	2.3
1	B	75	TYR	2.3
2	C	105	TYR	2.3
2	C	211	SER	2.3
1	B	272	TRP	2.3
2	E	196	TRP	2.3
1	B	181	GLY	2.3
1	B	79	LEU	2.3
1	A	72	ALA	2.3
1	B	39	ALA	2.3
1	B	122	VAL	2.3
1	B	357	PHE	2.3
1	B	165	ILE	2.2
1	B	400	ALA	2.2
1	A	31	THR	2.2
1	B	445	TYR	2.2
1	B	136	LEU	2.2
1	B	265	PHE	2.2
1	B	373	MET	2.2
3	D	68	THR	2.2
3	D	40	GLY	2.2
3	D	92	SER	2.2
3	D	176	SER	2.2
2	E	200	THR	2.2
1	A	431	GLY	2.2
2	C	172	HIS	2.2
1	A	390	ALA	2.2
1	B	230	ARG	2.2
1	A	30	LYS	2.2
3	D	102	LYS	2.2
1	B	48	LEU	2.2
1	B	198	LEU	2.2
2	C	44	GLY	2.2
2	C	84	SER	2.2
2	E	219	VAL	2.2
3	D	197	HIS	2.2
3	F	145	VAL	2.2
3	F	202	SER	2.2
2	C	70	ILE	2.2
1	B	432	ALA	2.1
1	A	167	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	286	GLY	2.1
1	A	69	VAL	2.1
1	B	69	VAL	2.1
2	C	73	ASP	2.1
1	B	17	ARG	2.1
1	B	147	ARG	2.1
1	B	312	THR	2.1
2	E	43	LYS	2.1
1	A	144	VAL	2.1
1	B	87	ALA	2.1
2	E	222	ALA	2.1
1	A	71	THR	2.1
1	A	251	THR	2.1
2	C	212	THR	2.1
2	C	5	LEU	2.1
1	B	287	ASN	2.1
1	A	299	GLY	2.1
1	B	142	GLY	2.1
1	A	450	ALA	2.1
1	A	455	LYS	2.1
3	D	163	THR	2.1
1	A	249	LEU	2.1
3	F	180	LEU	2.1
1	B	191	ASN	2.1
1	B	135	GLY	2.1
1	A	402	ILE	2.1
1	B	261	ILE	2.1
1	A	376	VAL	2.1
2	C	2	VAL	2.1
1	A	282	ARG	2.0
1	B	29	ASP	2.0
1	B	205	ARG	2.0
3	D	210	ARG	2.0
1	A	349	SER	2.0
1	B	297	ALA	2.0
2	C	43	LYS	2.0
1	A	254	LEU	2.0
1	A	215	ILE	2.0
1	A	94	TYR	2.0
1	A	130	VAL	2.0
1	B	236	VAL	2.0
2	E	32	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	362	ALA	2.0
1	B	55	LYS	2.0
3	D	71	SER	2.0
1	A	434	LEU	2.0
1	A	429	GLY	2.0
1	A	17	ARG	2.0
1	A	127	VAL	2.0
1	B	100	TYR	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 [i](#)

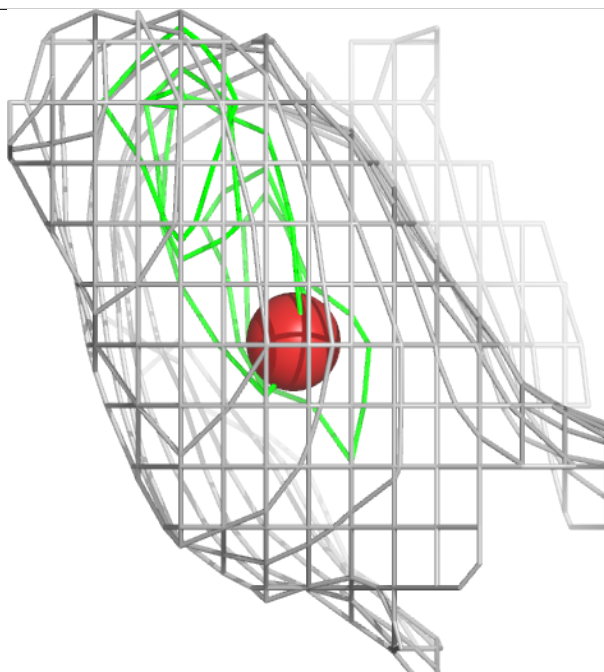
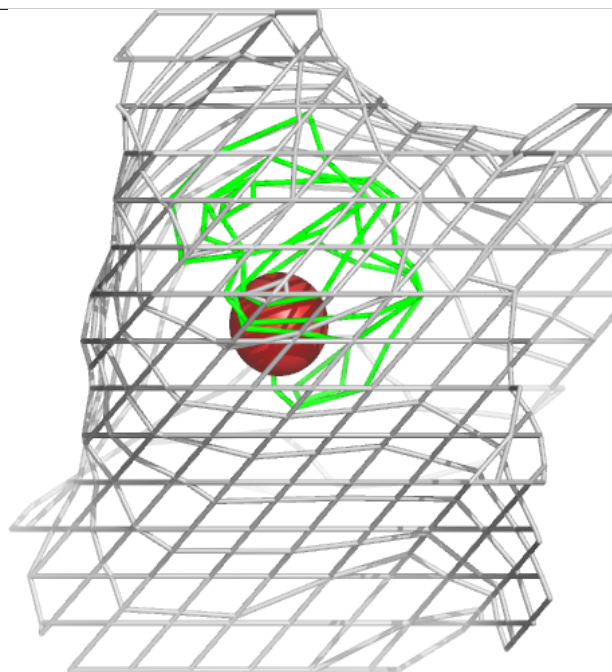
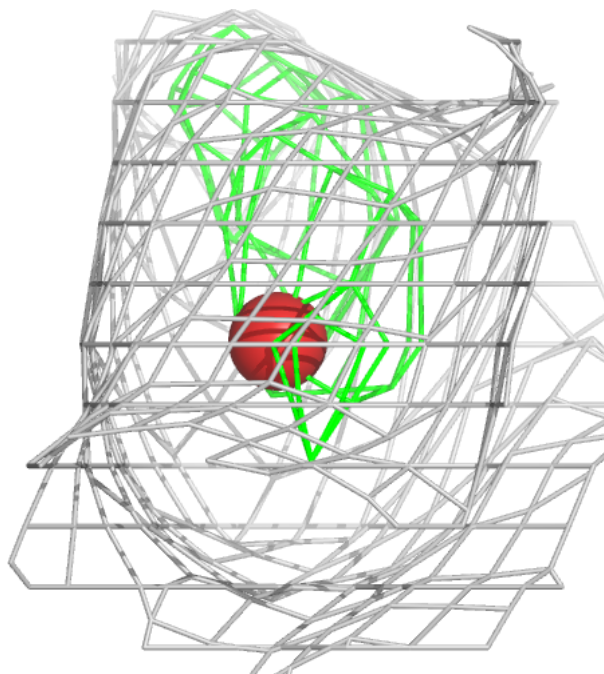
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BR	B	503	1/1	0.83	0.25	161,161,161,161	0
4	BR	B	502	1/1	0.86	0.19	141,141,141,141	0
4	BR	A	503	1/1	0.92	0.20	168,168,168,168	0
4	BR	A	502	1/1	0.94	0.16	123,123,123,123	0
4	BR	B	501	1/1	0.94	0.12	118,118,118,118	0
4	BR	A	501	1/1	0.97	0.12	125,125,125,125	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.

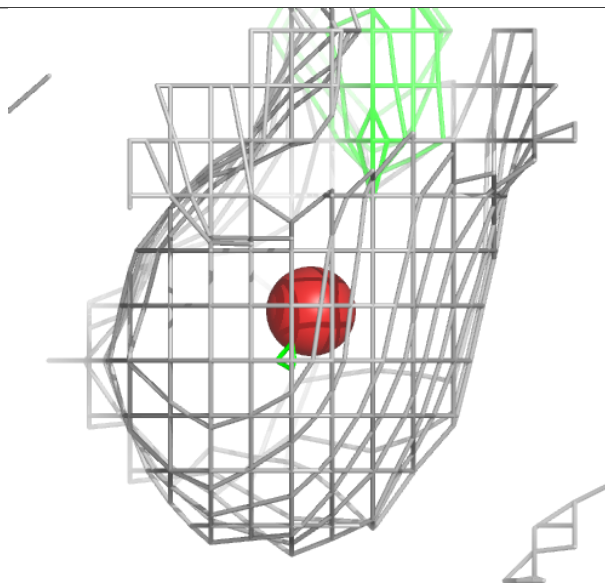
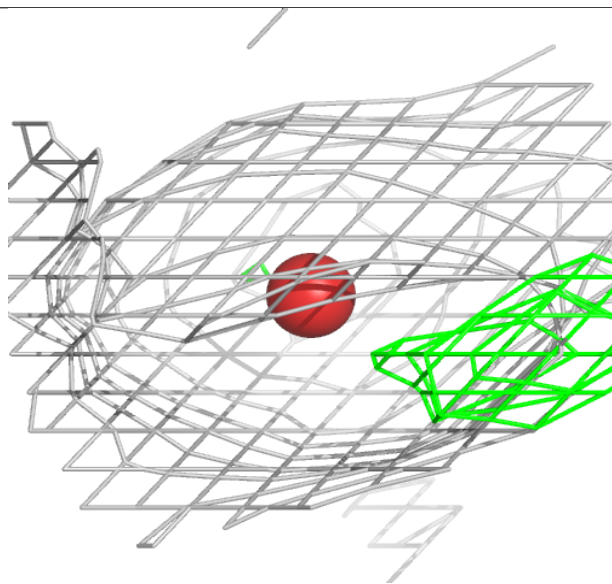
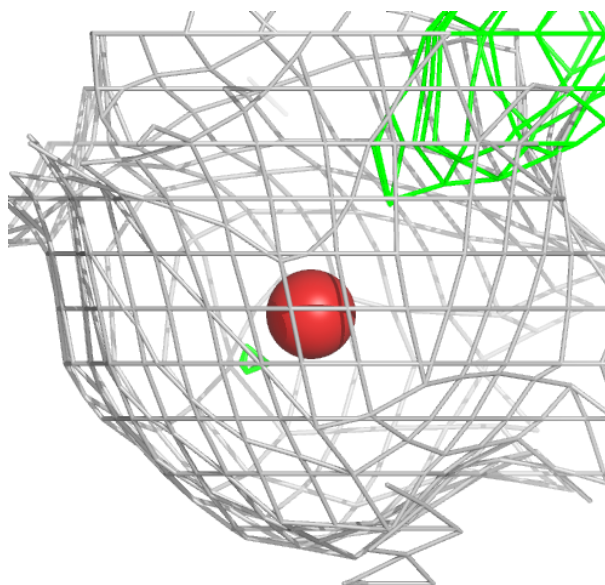
Electron density around BR B 503:

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



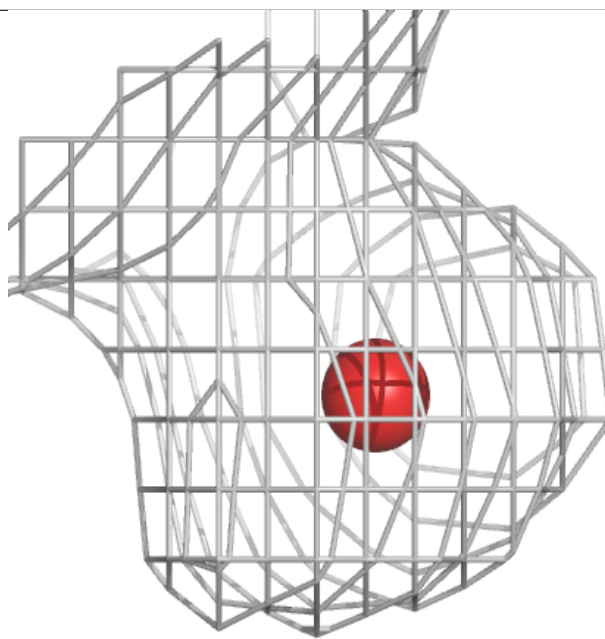
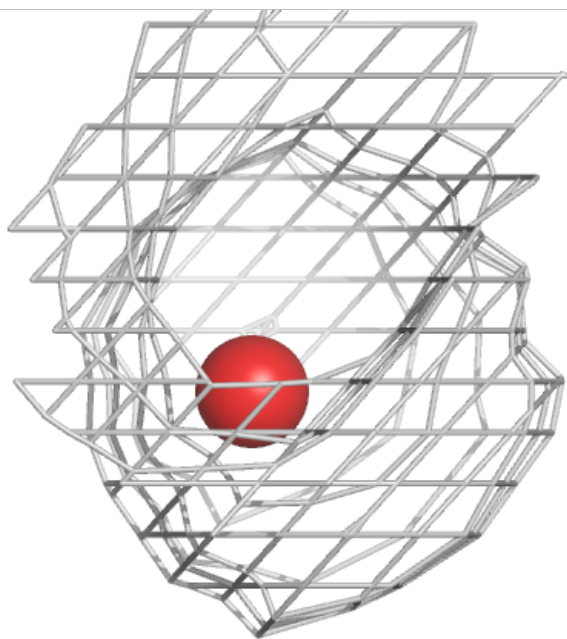
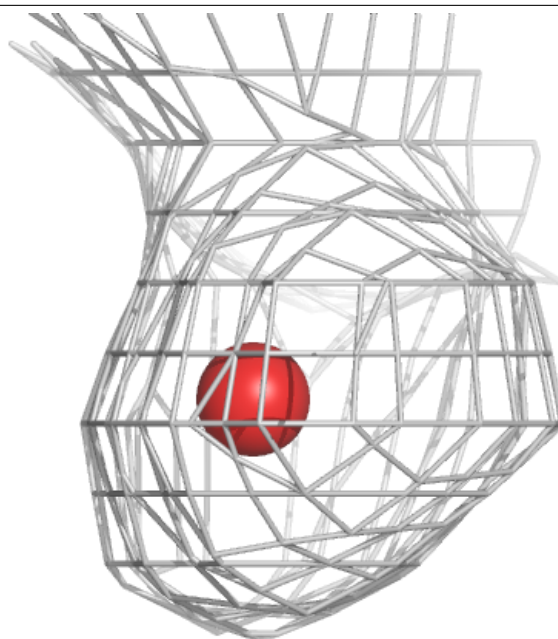
Electron density around BR B 502:

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



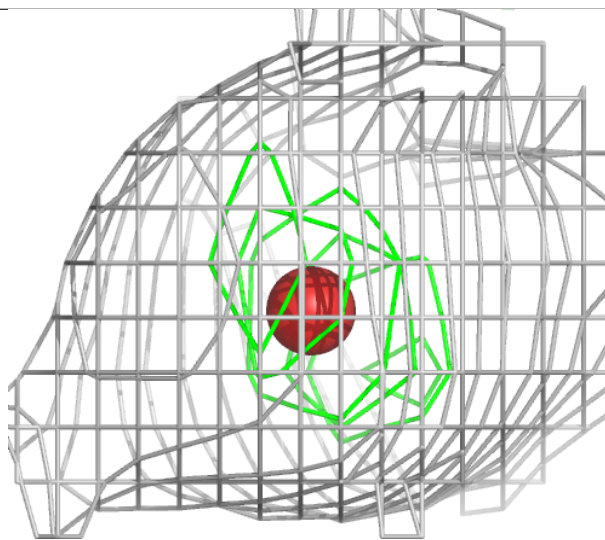
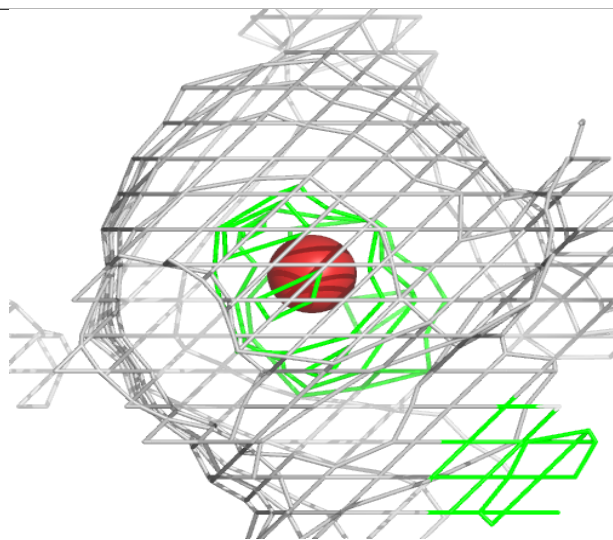
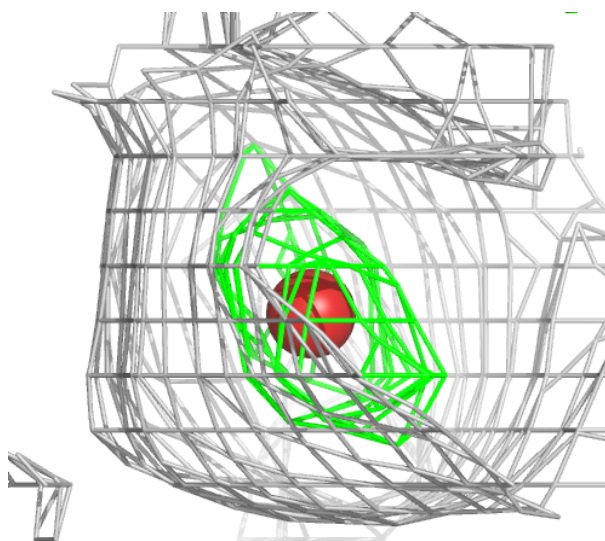
Electron density around BR A 503:

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



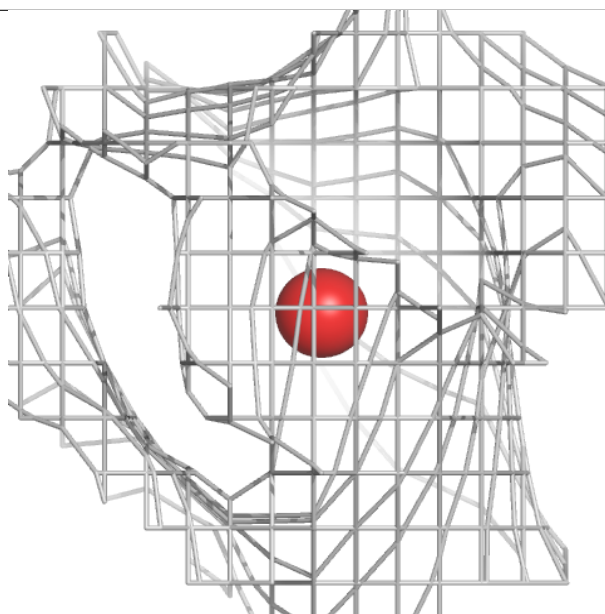
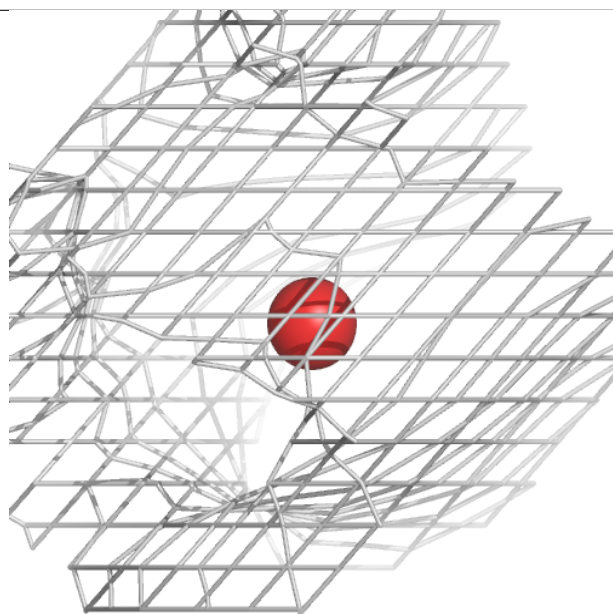
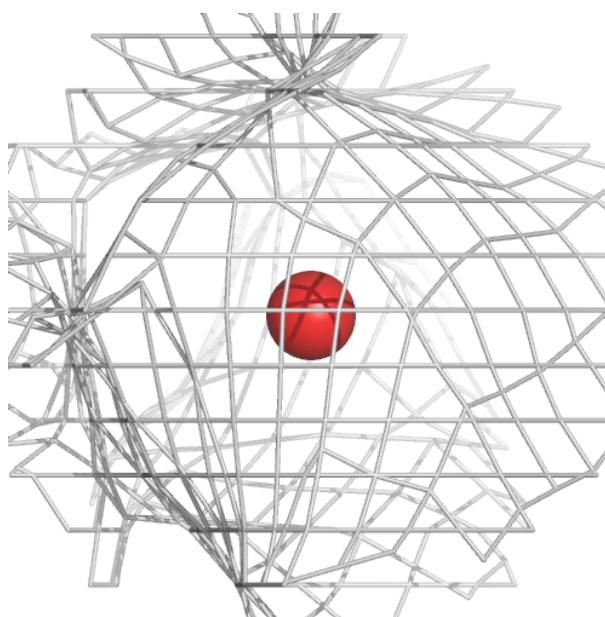
Electron density around BR A 502:

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and green (positive)



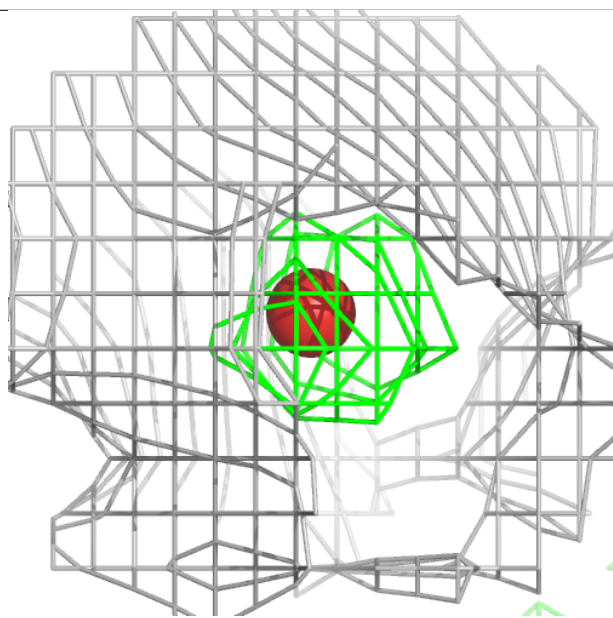
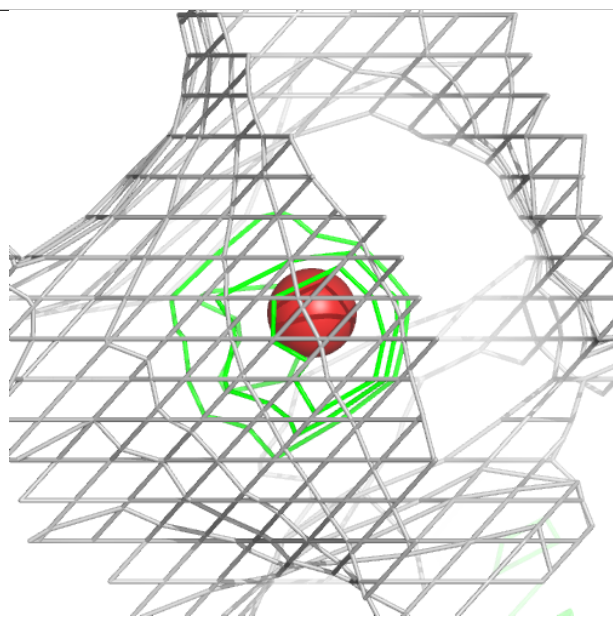
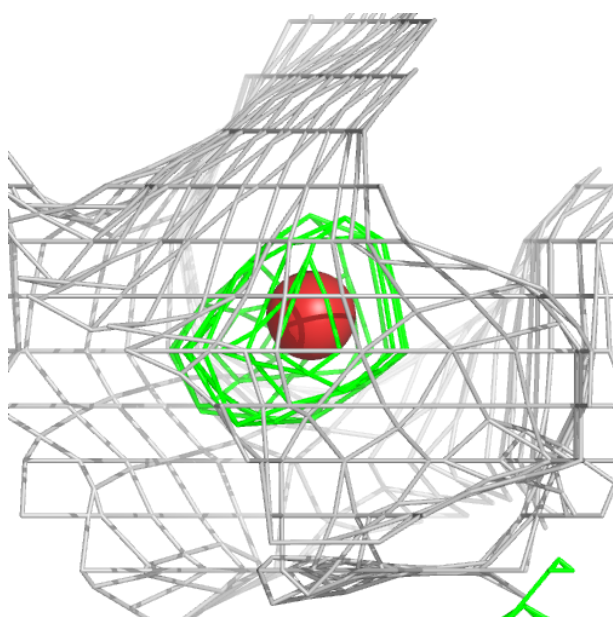
Electron density around BR B 501:

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



Electron density around BR 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.