



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:52 PM UTC

PDB ID : 8BOZ / pdb_00008boz
Title : structure of the Adherent-Invasive Escherichia coli Tle3/Tli3 T6SS effector/immunity complex
Authors : Cambillau, C.; Roussel, A.
Deposited on : 2022-11-15
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

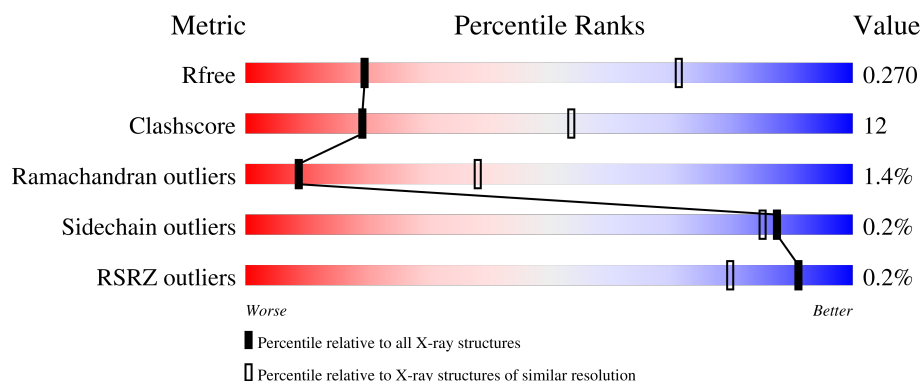
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	658	58% 23% • 18%
1	C	658	57% 22% 19%
1	E	658	63% 20% • 16%
1	G	658	66% 18% • 15%
1	I	658	63% 19% • 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	658	
1	M	658	
1	O	658	
2	B	274	
2	D	274	
2	F	274	
2	H	274	
2	J	274	
2	L	274	
2	N	274	
2	P	274	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45234 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 Transmembrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4072	2577	705	781	9			
1	C	530	Total	C	N	O	S	0	0	0
			3989	2529	681	770	9			
1	E	553	Total	C	N	O	S	0	0	0
			4127	2614	710	794	9			
1	G	558	Total	C	N	O	S	0	0	0
			4143	2619	713	802	9			
1	I	543	Total	C	N	O	S	0	0	0
			4042	2559	698	776	9			
1	K	546	Total	C	N	O	S	0	0	0
			4079	2580	703	787	9			
1	M	530	Total	C	N	O	S	0	0	0
			3978	2519	686	764	9			
1	O	521	Total	C	N	O	S	0	0	0
			3900	2466	672	754	8			

- Molecule 2 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1655	1051	281	313	10			
2	D	210	Total	C	N	O	S	0	0	0
			1615	1023	278	304	10			
2	F	213	Total	C	N	O	S	0	0	0
			1628	1032	277	309	10			
2	H	211	Total	C	N	O	S	0	0	0
			1609	1020	273	306	10			
2	J	216	Total	C	N	O	S	0	0	0
			1651	1043	283	315	10			
2	L	206	Total	C	N	O	S	0	0	0
			1586	1004	273	299	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	206	Total	C	N	O	S	0	0	0
			1580	1001	271	298	10			
2	P	204	Total	C	N	O	S	0	0	0
			1572	994	271	297	10			

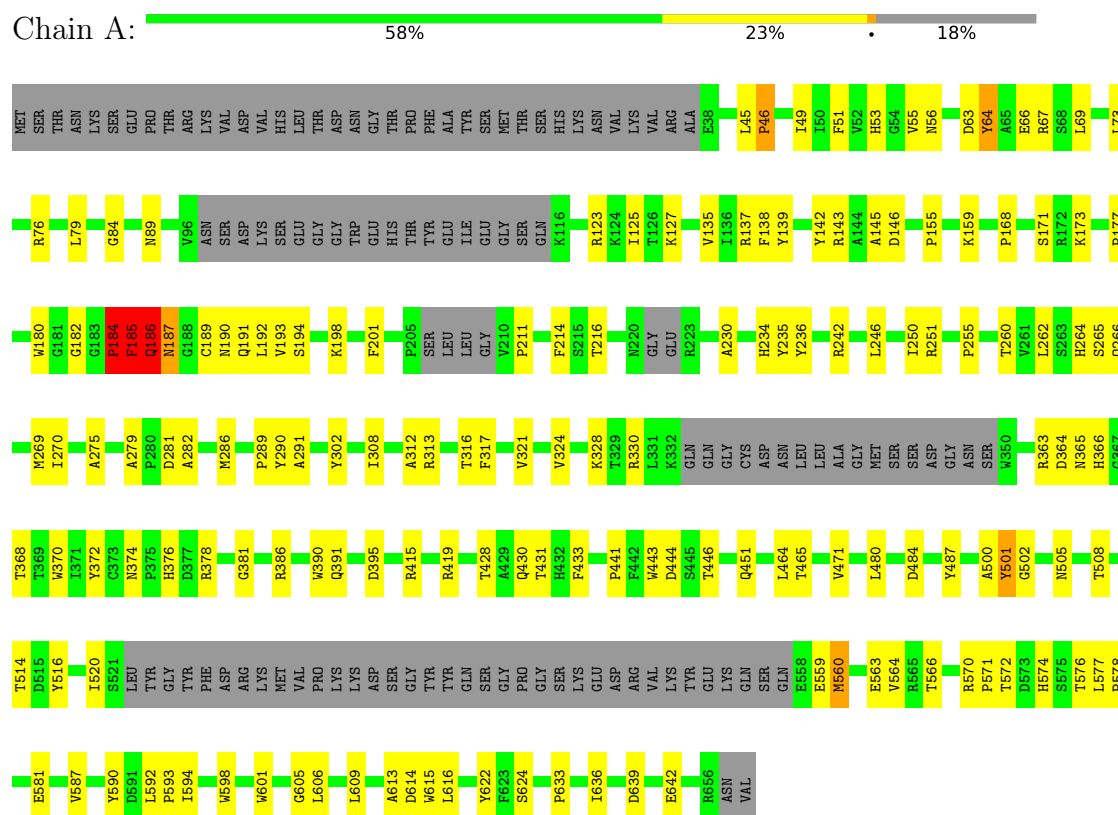
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		

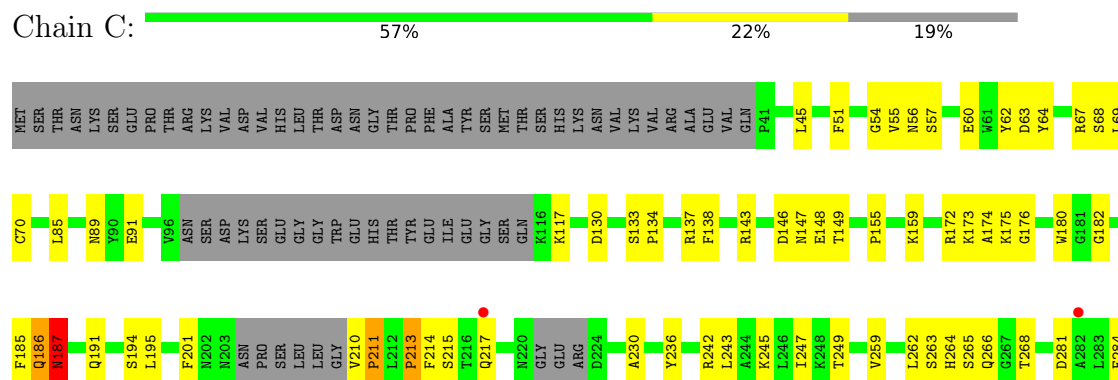
3 Residue-property plots

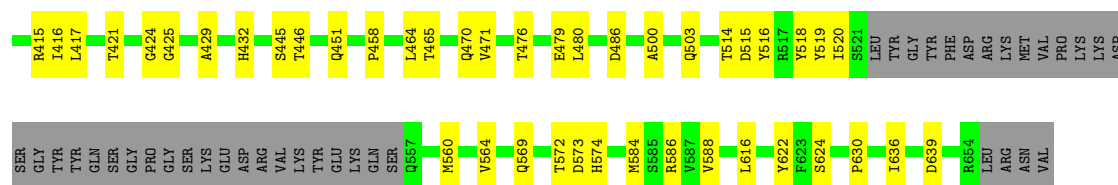
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



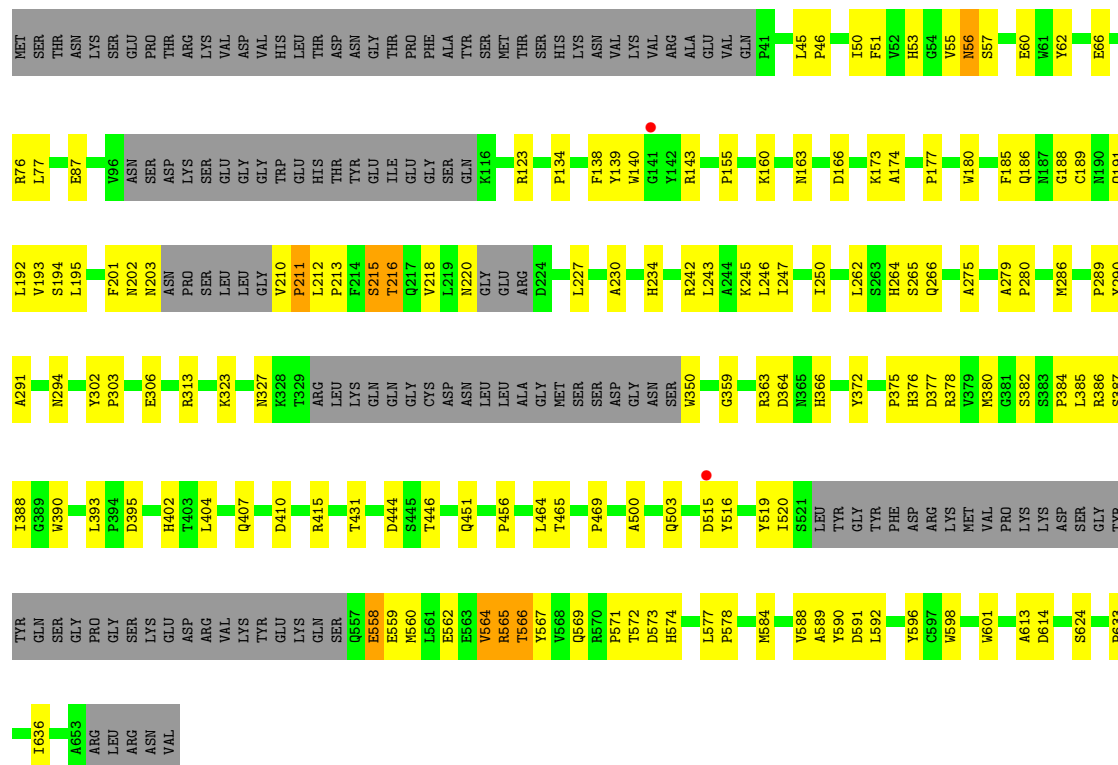
• Molecule 1: Transmembrane protein





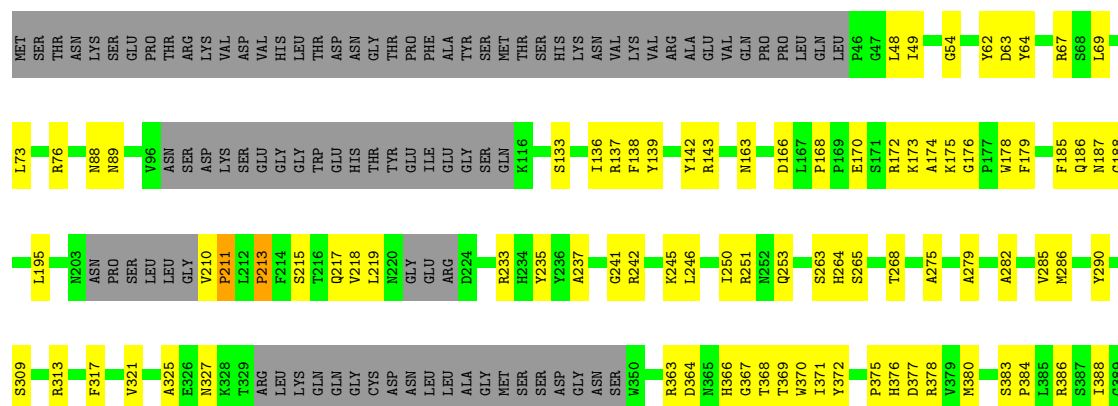
- Molecule 1: Transmembrane protein

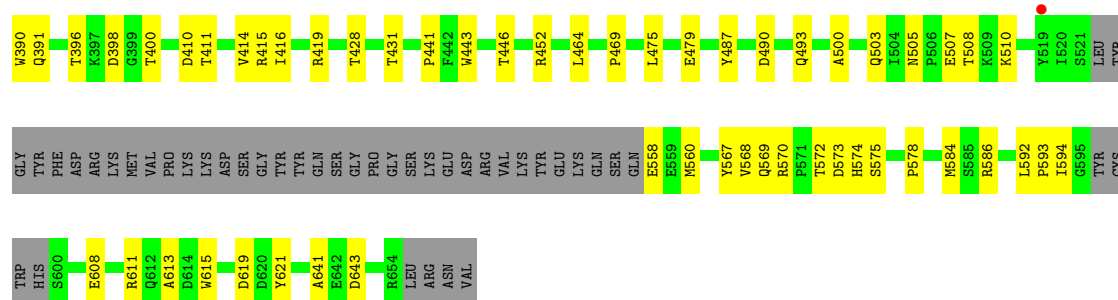
Chain M: 59% 21% 19%



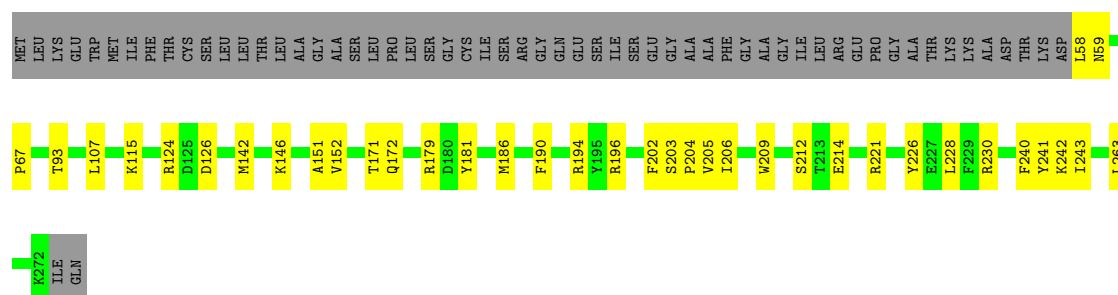
- Molecule 1: Transmembrane protein

Chain O: 58% 21% 21%

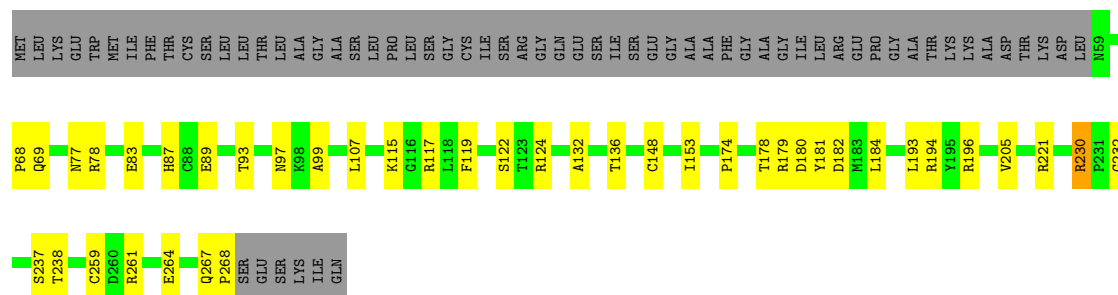




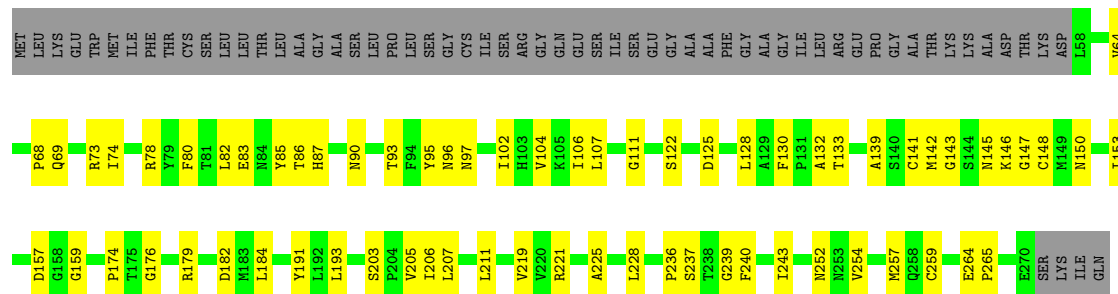
- Molecule 2: Lipoprotein



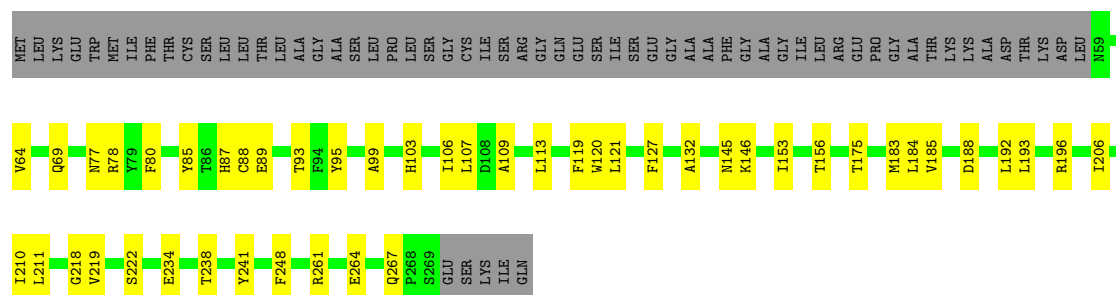
- Molecule 2: Lipoprotein



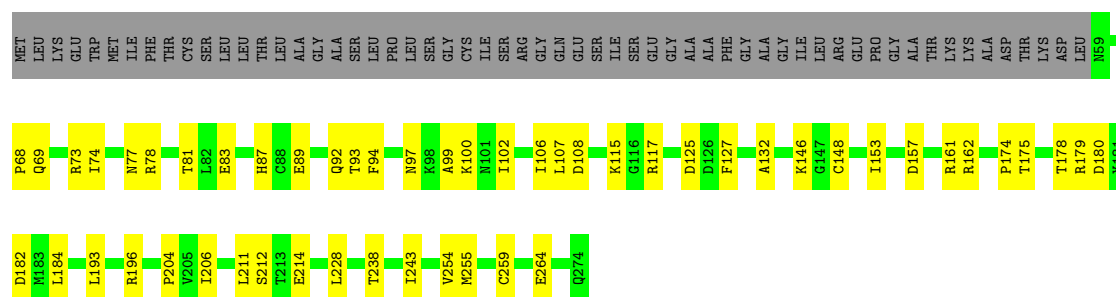
- Molecule 2: Lipoprotein



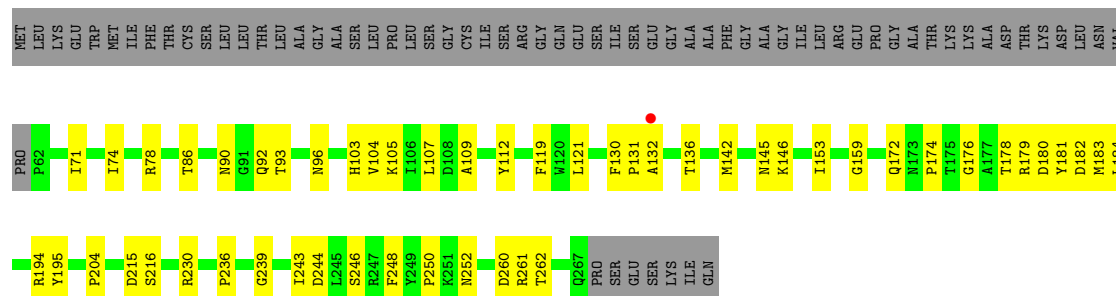
• Molecule 2: Lipoprotein

Chain H:  60% 17% 23%

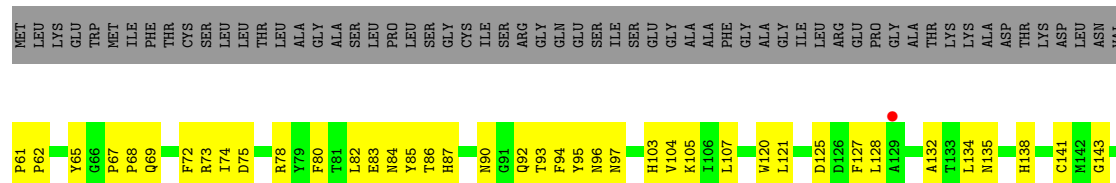
• Molecule 2: Lipoprotein

Chain J:  60% 19% 21%

• Molecule 2: Lipoprotein

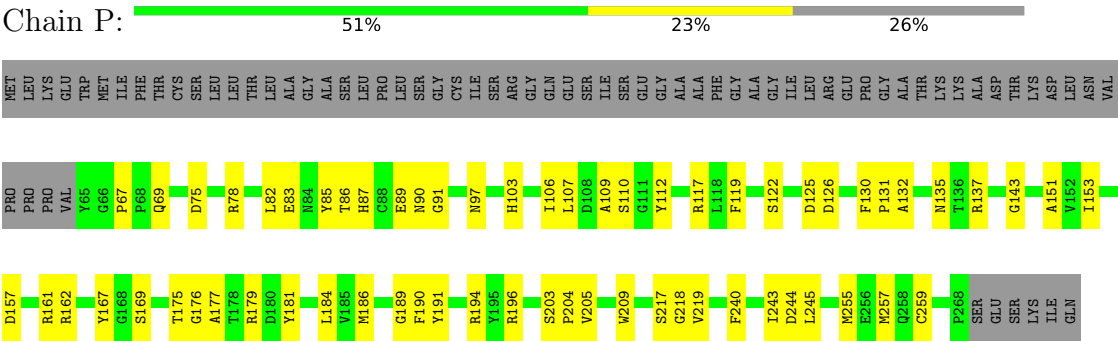
Chain L:  56% 19% 25%

• Molecule 2: Lipoprotein

Chain N:  54% 21% 25%



● Molecule 2: Lipoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.86Å 449.07Å 116.23Å 90.00° 93.18° 90.00°	Depositor
Resolution (Å)	48.74 – 3.60 48.74 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.74-3.60) 98.9 (48.74-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.233 , 0.268 0.234 , 0.270	Depositor DCC
R_{free} test set	3949 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	45234	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/4188	0.37	2/5736 (0.0%)
1	C	0.18	0/4102	0.39	2/5618 (0.0%)
1	E	0.17	0/4246	0.37	0/5819
1	G	0.18	0/4259	0.41	1/5838 (0.0%)
1	I	0.15	0/4157	0.39	0/5700
1	K	0.15	0/4193	0.33	0/5745
1	M	0.17	0/4091	0.34	0/5604
1	O	0.16	0/4008	0.32	0/5486
2	B	0.11	0/1699	0.31	0/2316
2	D	0.14	0/1657	0.32	0/2258
2	F	0.11	0/1670	0.29	0/2277
2	H	0.10	0/1651	0.28	0/2252
2	J	0.12	0/1693	0.30	0/2307
2	L	0.10	0/1626	0.27	0/2212
2	N	0.10	0/1621	0.29	0/2208
2	P	0.11	0/1611	0.34	0/2191
All	All	0.15	0/46472	0.35	5/63567 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ASN	CA-C-N	-7.34	114.37	120.98
1	C	187	ASN	C-N-CA	-7.34	114.37	120.98
1	A	187	ASN	CA-C-N	-6.08	112.85	121.54
1	A	187	ASN	C-N-CA	-6.08	112.85	121.54
1	G	265	SER	CB-CA-C	-5.20	110.56	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	TYR	Peptide

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	4072	0	3708	118	0
1	C	3989	0	3645	117	0
1	E	4127	0	3709	92	0
1	G	4143	0	3713	70	0
1	I	4042	0	3646	82	0
1	K	4079	0	3693	105	0
1	M	3978	0	3627	100	0
1	O	3900	0	3540	97	0
2	B	1655	0	1537	26	0
2	D	1615	0	1505	30	0
2	F	1628	0	1510	44	0
2	H	1609	0	1488	28	0
2	J	1651	0	1525	36	0
2	L	1586	0	1477	30	0
2	N	1580	0	1465	35	0
2	P	1572	0	1460	46	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	1	0	0	0	0
3	O	1	0	0	0	0
All	All	45234	0	41248	1011	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1011) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:331:LEU:HD12	1:K:366:HIS:CD2	1.36	1.57
1:K:331:LEU:CD1	1:K:366:HIS:CD2	2.05	1.38
1:K:331:LEU:CD1	1:K:366:HIS:HD2	1.33	1.37
1:C:185:PHE:CZ	1:C:217:GLN:NE2	2.19	1.10
1:K:258:THR:HG22	1:K:331:LEU:HD11	1.48	0.96
1:K:258:THR:HG22	1:K:331:LEU:CD1	1.93	0.96
1:O:173:LYS:H	1:O:178:TRP:HE1	1.17	0.93
1:C:185:PHE:HZ	1:C:217:GLN:HE22	1.10	0.92
1:A:55:VAL:HG11	1:A:185:PHE:HA	1.56	0.88
1:K:331:LEU:HD13	1:K:366:HIS:CD2	2.08	0.87
1:C:185:PHE:CE1	1:C:217:GLN:NE2	2.42	0.86
1:C:211:PRO:HD2	1:C:213:PRO:HG3	1.57	0.86
1:G:364:ASP:OD1	1:G:366:HIS:ND1	2.09	0.86
1:G:76:ARG:NH1	1:G:362:GLU:OE2	2.10	0.83
1:K:364:ASP:OD1	1:K:366:HIS:ND1	2.11	0.82
1:K:118:TRP:CD1	1:K:514:THR:HG1	1.97	0.82
1:O:211:PRO:HG2	1:O:213:PRO:HG3	1.62	0.81
1:A:55:VAL:CG1	1:A:185:PHE:HA	2.11	0.80
1:C:215:SER:HB2	1:C:572:THR:HG21	1.65	0.78
1:E:514:THR:OG1	2:F:146:LYS:NZ	2.17	0.78
1:C:117:LYS:HG3	1:C:517:ARG:HD3	1.65	0.77
1:G:386:ARG:NH2	1:G:456:PRO:O	2.18	0.77
1:K:173:LYS:H	1:K:178:TRP:HE1	1.32	0.77
1:E:55:VAL:HG11	1:E:185:PHE:HA	1.67	0.76
1:E:265:SER:OG	1:E:574:HIS:NE2	2.19	0.76
2:P:69:GLN:NE2	2:P:259:CYS:SG	2.55	0.75
1:C:55:VAL:CG1	1:C:185:PHE:HA	2.15	0.75
1:G:507:GLU:HG2	2:H:109:ALA:HB2	1.67	0.75
2:N:97:ASN:ND2	2:N:125:ASP:OD2	2.20	0.74
1:C:289:PRO:HA	1:C:380:MET:HE1	1.68	0.74
1:E:366:HIS:HE1	1:E:595:GLY:HA3	1.53	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:67:ARG:NH2	2:J:180:ASP:OD2	2.20	0.74
1:O:163:ASN:HB3	1:O:166:ASP:HB2	1.68	0.73
2:D:136:THR:HG22	2:D:174:PRO:HD2	1.69	0.73
1:K:258:THR:HG22	1:K:331:LEU:HD13	1.71	0.73
1:I:262:LEU:HD12	1:I:286:MET:HE3	1.71	0.73
1:K:312:ALA:HB2	1:K:639:ASP:HB2	1.71	0.73
1:K:67:ARG:NH2	2:L:180:ASP:OD2	2.22	0.72
1:K:331:LEU:HD12	1:K:366:HIS:HD2	0.69	0.72
2:H:77:ASN:HD21	2:H:99:ALA:HB2	1.55	0.72
1:O:268:THR:HB	1:O:285:VAL:HG23	1.70	0.72
2:D:69:GLN:NE2	2:D:259:CYS:SG	2.64	0.71
1:C:185:PHE:HZ	1:C:217:GLN:NE2	1.73	0.70
1:I:363:ARG:NH2	1:I:591:ASP:OD1	2.26	0.69
1:C:446:THR:HG23	1:C:451:GLN:HB3	1.75	0.69
1:O:309:SER:HA	1:O:641:ALA:HB2	1.74	0.68
2:H:87:HIS:HA	2:H:264:GLU:HG2	1.74	0.68
1:K:191:GLN:NE2	1:K:194:SER:OG	2.26	0.68
1:A:64:TYR:OH	1:A:581:GLU:OE1	2.10	0.67
1:A:514:THR:OG1	2:B:146:LYS:NZ	2.27	0.67
1:C:191:GLN:NE2	1:C:194:SER:OG	2.28	0.67
2:F:106:ILE:HG22	2:F:107:LEU:HD12	1.74	0.67
2:J:77:ASN:HD21	2:J:99:ALA:HB2	1.59	0.67
2:P:106:ILE:O	2:P:162:ARG:NH2	2.26	0.67
1:A:291:ALA:O	1:A:313:ARG:NH1	2.28	0.67
1:A:146:ASP:HA	1:A:173:LYS:HZ1	1.60	0.66
1:I:191:GLN:NE2	1:I:194:SER:OG	2.27	0.66
1:A:143:ARG:HE	1:A:177:PRO:HB3	1.59	0.66
1:O:608:GLU:HB2	1:O:611:ARG:HH21	1.59	0.66
1:A:633:PRO:HD2	1:A:636:ILE:HD12	1.78	0.66
1:G:633:PRO:HD2	1:G:636:ILE:HD12	1.77	0.66
2:H:93:THR:HB	2:H:107:LEU:HB3	1.78	0.66
2:P:184:LEU:HB3	2:P:191:TYR:HB2	1.78	0.66
1:K:265:SER:O	1:K:268:THR:HG22	1.96	0.66
1:G:312:ALA:HB2	1:G:639:ASP:HB2	1.77	0.65
1:E:294:ASN:OD1	1:E:313:ARG:NH2	2.28	0.65
1:E:395:ASP:OD1	1:E:465:THR:OG1	2.12	0.65
1:K:143:ARG:NH1	1:K:624:SER:O	2.29	0.65
1:I:185:PHE:CE1	1:I:214:PHE:HB2	2.31	0.65
2:N:104:VAL:HG21	2:N:159:GLY:HA3	1.78	0.65
1:A:73:LEU:HD11	1:A:592:LEU:HD12	1.79	0.65
1:C:486:ASP:OD1	1:C:487:TYR:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:571:PRO:HB3	2:F:143:GLY:HA3	1.79	0.64
1:A:193:VAL:HG11	1:A:308:ILE:HD11	1.79	0.64
1:E:190:ASN:O	1:E:313:ARG:NH1	2.31	0.64
1:K:211:PRO:HD2	1:K:213:PRO:HG3	1.79	0.64
1:C:505:ASN:HB3	1:C:508:THR:HG22	1.78	0.64
1:G:321:VAL:HG21	1:G:412:LEU:HD12	1.80	0.64
1:M:264:HIS:CD2	1:M:578:PRO:HG3	2.33	0.64
1:E:365:ASN:HB2	1:E:593:PRO:HA	1.78	0.64
1:G:191:GLN:NE2	1:G:306:GLU:O	2.31	0.64
1:G:514:THR:HB	2:H:146:LYS:HE2	1.80	0.64
2:J:204:PRO:HG2	2:J:243:ILE:HD12	1.79	0.64
1:M:380:MET:HE2	1:M:387:SER:HB3	1.80	0.64
1:M:53:HIS:HE1	1:M:139:TYR:HA	1.63	0.64
1:O:188:GLY:O	1:O:233:ARG:NH2	2.31	0.64
1:A:316:THR:HG23	1:A:636:ILE:HA	1.79	0.64
1:I:632:ILE:HG21	1:I:638:GLN:HE21	1.62	0.64
1:C:368:THR:OG1	1:C:370:TRP:NE1	2.32	0.63
1:C:55:VAL:HG11	1:C:185:PHE:HA	1.80	0.63
2:H:183:MET:HE2	2:H:192:LEU:HD21	1.81	0.63
1:O:62:TYR:HB3	1:O:137:ARG:HE	1.63	0.63
2:F:132:ALA:HB2	2:F:153:ILE:HG12	1.81	0.63
1:A:67:ARG:HH21	2:B:194:ARG:HE	1.46	0.63
1:C:262:LEU:HD21	1:C:584:MET:HE1	1.81	0.63
1:E:185:PHE:HD1	1:E:214:PHE:HB2	1.63	0.63
1:E:366:HIS:CE1	1:E:595:GLY:HA3	2.33	0.63
1:A:560:MET:O	1:A:564:VAL:HG23	1.99	0.63
1:C:67:ARG:HH12	2:D:194:ARG:HH21	1.46	0.63
1:O:137:ARG:HB3	1:O:139:TYR:HE1	1.63	0.62
1:E:216:THR:HA	1:E:569:GLN:NE2	2.14	0.62
2:N:68:PRO:HB3	2:N:83:GLU:HG2	1.82	0.62
1:C:446:THR:HG22	1:C:452:ARG:HG2	1.81	0.62
1:G:173:LYS:H	1:G:178:TRP:HE1	1.45	0.62
2:J:97:ASN:ND2	2:J:125:ASP:OD2	2.33	0.62
1:A:446:THR:HG23	1:A:451:GLN:HB3	1.82	0.62
1:E:191:GLN:NE2	1:E:194:SER:OG	2.33	0.62
1:C:378:ARG:NH1	1:C:444:ASP:OD1	2.33	0.62
1:A:198:LYS:HD3	1:A:234:HIS:NE2	2.14	0.62
1:C:356:THR:HG22	1:C:357:HIS:H	1.64	0.62
1:K:185:PHE:CD1	1:K:214:PHE:HD2	2.18	0.62
1:M:291:ALA:O	1:M:313:ARG:NH1	2.33	0.62
1:M:404:LEU:HA	1:M:407:GLN:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ARG:NH2	1:A:279:ALA:O	2.33	0.62
1:G:40:GLN:HB2	1:G:41:PRO:HD3	1.82	0.62
2:L:86:THR:HG1	2:L:90:ASN:HD21	1.48	0.62
1:G:145:ALA:HB3	1:G:148:GLU:HB2	1.81	0.61
1:I:446:THR:HG23	1:I:451:GLN:HB3	1.81	0.61
2:N:93:THR:HB	2:N:107:LEU:HB2	1.81	0.61
2:N:193:LEU:HG	2:N:206:ILE:HG12	1.82	0.61
1:K:215:SER:O	1:K:569:GLN:NE2	2.33	0.61
1:E:363:ARG:NH2	1:E:591:ASP:OD1	2.33	0.61
1:I:65:ALA:HB1	1:I:584:MET:HE3	1.81	0.61
1:E:572:THR:O	1:E:574:HIS:N	2.32	0.61
1:K:368:THR:OG1	1:K:370:TRP:NE1	2.34	0.61
1:K:55:VAL:HG23	1:K:266:GLN:HG2	1.82	0.61
1:K:515:ASP:OD2	2:L:146:LYS:NZ	2.23	0.61
1:C:321:VAL:HG21	1:C:412:LEU:HD12	1.81	0.61
1:C:185:PHE:CD1	1:C:214:PHE:HB2	2.36	0.60
1:M:364:ASP:OD1	1:M:366:HIS:ND1	2.34	0.60
2:N:132:ALA:HB2	2:N:153:ILE:HG12	1.83	0.60
1:A:63:ASP:OD1	1:A:137:ARG:NH1	2.33	0.60
1:E:312:ALA:HB2	1:E:639:ASP:HB2	1.81	0.60
2:D:119:PHE:HB2	2:D:184:LEU:HD23	1.81	0.60
1:K:321:VAL:HG21	1:K:412:LEU:HD12	1.83	0.60
1:K:560:MET:O	1:K:564:VAL:HG23	2.02	0.60
1:I:358:ASN:HA	1:M:359:GLY:HA3	1.83	0.60
1:E:378:ARG:NH1	1:E:444:ASP:OD1	2.35	0.60
1:A:282:ALA:HB2	1:A:593:PRO:HG3	1.83	0.60
1:A:364:ASP:OD1	1:A:366:HIS:ND1	2.34	0.60
1:E:377:ASP:OD1	1:E:574:HIS:ND1	2.35	0.60
1:M:584:MET:HA	1:M:588:VAL:HB	1.83	0.60
2:J:117:ARG:NH2	2:J:182:ASP:OD2	2.32	0.60
1:K:56:ASN:HA	1:K:180:TRP:CH2	2.36	0.60
1:O:363:ARG:HD2	1:O:469:PRO:HG2	1.85	0.59
1:I:220:ASN:HB2	1:I:450:LEU:HD21	1.84	0.59
1:K:53:HIS:O	1:K:140:TRP:NE1	2.36	0.59
1:A:123:ARG:NH1	1:A:614:ASP:OD1	2.36	0.59
1:M:218:VAL:HG12	1:M:220:ASN:H	1.68	0.59
2:J:93:THR:HB	2:J:107:LEU:HB2	1.85	0.59
1:O:493:GLN:HB3	1:O:503:GLN:HE22	1.67	0.59
1:G:572:THR:O	1:G:574:HIS:N	2.32	0.59
2:L:107:LEU:HG	2:L:109:ALA:H	1.67	0.59
1:M:415:ARG:NH2	1:M:469:PRO:O	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:475:LEU:HD23	1:O:586:ARG:HH21	1.68	0.59
1:A:145:ALA:O	1:A:173:LYS:NZ	2.35	0.58
2:F:69:GLN:NE2	2:F:259:CYS:SG	2.76	0.58
1:A:185:PHE:C	1:A:187:ASN:H	2.11	0.58
1:C:215:SER:CB	1:C:572:THR:HG21	2.32	0.58
2:D:89:GLU:OE2	2:D:261:ARG:NH2	2.36	0.58
1:K:211:PRO:O	1:K:384:PRO:HG2	2.02	0.58
1:K:476:THR:HG23	1:K:479:GLU:H	1.68	0.58
2:B:206:ILE:HD13	2:B:228:LEU:HD12	1.84	0.58
1:K:211:PRO:O	1:K:213:PRO:HD3	2.02	0.58
1:C:195:LEU:HD22	1:C:236:TYR:HB3	1.83	0.58
1:E:282:ALA:HB3	1:E:593:PRO:HG3	1.85	0.58
2:J:69:GLN:NE2	2:J:259:CYS:SG	2.75	0.58
1:C:91:GLU:OE1	2:D:221:ARG:NH2	2.37	0.58
1:M:203:ASN:ND2	1:M:227:LEU:O	2.36	0.58
2:H:196:ARG:NH2	2:H:238:THR:O	2.35	0.58
2:F:107:LEU:HD21	2:F:132:ALA:HA	1.86	0.58
1:M:56:ASN:HB2	1:M:180:TRP:HE1	1.69	0.58
1:O:264:HIS:HE1	1:O:574:HIS:CD2	2.22	0.58
1:O:508:THR:HB	2:P:151:ALA:HB3	1.86	0.58
1:A:191:GLN:NE2	1:A:194:SER:OG	2.36	0.57
2:F:93:THR:HG21	2:F:111:GLY:H	1.68	0.57
1:I:600:SER:O	1:I:601:TRP:HB2	2.04	0.57
2:P:167:TYR:HE2	2:P:181:TYR:CE2	2.22	0.57
1:C:185:PHE:HD1	1:C:214:PHE:HB2	1.69	0.57
1:E:264:HIS:CD2	1:E:578:PRO:HG3	2.39	0.57
1:C:364:ASP:OD1	1:C:366:HIS:ND1	2.37	0.57
1:M:76:ARG:HG2	1:M:77:LEU:HD12	1.86	0.57
2:P:97:ASN:ND2	2:P:125:ASP:OD2	2.38	0.57
2:P:132:ALA:HB2	2:P:153:ILE:HG12	1.87	0.57
2:B:124:ARG:NH2	2:B:126:ASP:OD2	2.37	0.57
2:J:132:ALA:HB2	2:J:153:ILE:HG12	1.87	0.57
1:K:331:LEU:HD13	1:K:366:HIS:NE2	2.20	0.57
2:L:119:PHE:HB2	2:L:184:LEU:HD23	1.86	0.57
1:A:46:PRO:HB3	1:A:598:TRP:CE2	2.40	0.57
1:E:89:ASN:HD22	2:F:205:VAL:HG11	1.69	0.57
1:K:446:THR:HG23	1:K:451:GLN:HB3	1.87	0.57
1:O:377:ASP:OD2	1:O:574:HIS:ND1	2.38	0.56
1:E:55:VAL:CG1	1:E:185:PHE:HA	2.34	0.56
2:F:211:LEU:HD23	2:F:219:VAL:HG12	1.87	0.56
1:I:218:VAL:HG12	1:I:220:ASN:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:210:VAL:N	1:M:211:PRO:HD3	2.21	0.56
2:H:80:PHE:HE1	2:H:106:ILE:HG13	1.70	0.56
1:I:129:GLY:O	2:J:196:ARG:NH1	2.37	0.56
1:I:487:TYR:HD2	1:I:490:ASP:HB3	1.71	0.56
1:M:500:ALA:HB3	1:M:503:GLN:HG3	1.87	0.56
1:O:572:THR:O	1:O:574:HIS:N	2.38	0.56
1:M:395:ASP:OD1	1:M:465:THR:HG23	2.05	0.56
2:N:149:MET:HE2	2:N:166:PRO:HB2	1.87	0.56
1:C:404:LEU:HA	1:C:407:GLN:HB2	1.87	0.56
1:G:501:TYR:CD1	1:G:516:TYR:HD1	2.23	0.56
1:E:246:LEU:O	1:E:250:ILE:HG13	2.06	0.56
1:K:572:THR:O	1:K:574:HIS:N	2.39	0.56
1:C:211:PRO:O	1:C:213:PRO:HD3	2.05	0.56
1:E:155:PRO:HG3	1:E:519:TYR:CE1	2.41	0.56
1:O:263:SER:O	1:O:286:MET:HB3	2.06	0.56
1:C:64:TYR:OH	1:C:581:GLU:OE1	2.20	0.56
1:I:589:ALA:HA	1:I:592:LEU:HD13	1.86	0.56
1:O:368:THR:OG1	1:O:370:TRP:NE1	2.39	0.56
1:A:312:ALA:HB2	1:A:639:ASP:HB2	1.88	0.56
1:I:285:VAL:HG23	1:I:371:ILE:HA	1.88	0.56
2:P:107:LEU:HD13	2:P:153:ILE:HG13	1.88	0.56
1:E:216:THR:HA	1:E:569:GLN:HE22	1.69	0.56
2:H:193:LEU:HG	2:H:206:ILE:HG12	1.88	0.56
2:L:176:GLY:HA2	2:L:179:ARG:HH11	1.71	0.56
1:M:386:ARG:NH1	1:M:456:PRO:O	2.37	0.56
2:B:212:SER:OG	2:B:214:GLU:HG2	2.05	0.55
1:A:185:PHE:CD2	1:A:214:PHE:HB2	2.41	0.55
2:B:58:LEU:HG	2:B:59:ASN:H	1.71	0.55
1:E:68:SER:HB2	1:E:584:MET:HB2	1.89	0.55
1:E:316:THR:O	1:E:320:ILE:HD12	2.06	0.55
1:O:428:THR:OG1	1:O:431:THR:OG1	2.19	0.55
2:P:196:ARG:HD2	2:P:205:VAL:HG23	1.88	0.55
1:A:55:VAL:HG23	1:A:266:GLN:HB3	1.87	0.55
1:A:190:ASN:HD22	1:A:313:ARG:HH12	1.55	0.55
2:B:202:PHE:HB3	2:B:241:TYR:CE1	2.41	0.55
1:O:63:ASP:OD2	2:P:169:SER:OG	2.17	0.55
2:B:67:PRO:HG2	2:B:263:LEU:HD23	1.88	0.55
1:G:247:ILE:HA	1:G:250:ILE:HD12	1.89	0.55
1:E:209:GLY:O	1:E:210:VAL:HB	2.05	0.55
1:I:572:THR:O	1:I:574:HIS:N	2.38	0.55
2:J:175:THR:O	2:J:178:THR:OG1	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:265:SER:OG	1:M:266:GLN:N	2.40	0.55
1:C:242:ARG:NH2	1:C:615:TRP:HB3	2.22	0.55
1:O:48:LEU:HD13	1:O:136:ILE:HD11	1.87	0.55
2:P:181:TYR:CE1	2:P:194:ARG:HB3	2.41	0.55
1:A:505:ASN:HB3	1:A:508:THR:HG22	1.88	0.55
1:E:70:CYS:O	1:E:74:ASN:ND2	2.40	0.55
1:K:395:ASP:OD1	1:K:465:THR:OG1	2.20	0.55
1:C:143:ARG:NH1	1:C:624:SER:O	2.40	0.55
1:C:376:HIS:HE1	1:C:419:ARG:HB3	1.72	0.55
1:K:185:PHE:HD1	1:K:214:PHE:HD2	1.52	0.55
1:M:53:HIS:CE1	1:M:140:TRP:H	2.24	0.55
2:L:236:PRO:HG2	2:L:239:GLY:H	1.72	0.54
1:E:420:ASN:HD22	1:E:438:ASP:HB3	1.72	0.54
1:M:123:ARG:NH1	1:M:614:ASP:OD1	2.40	0.54
1:A:428:THR:OG1	1:A:431:THR:OG1	2.21	0.54
1:G:350:TRP:CZ2	1:G:362:GLU:HG2	2.42	0.54
2:H:132:ALA:HB2	2:H:153:ILE:HG12	1.89	0.54
1:I:560:MET:O	1:I:564:VAL:HG23	2.07	0.54
1:O:396:THR:HG1	1:O:400:THR:HG1	1.55	0.54
2:P:90:ASN:O	2:P:110:SER:OG	2.25	0.54
1:C:572:THR:C	1:C:574:HIS:H	2.16	0.54
1:I:281:ASP:O	1:I:367:GLY:N	2.37	0.54
2:F:207:LEU:HD22	2:F:221:ARG:HH21	1.73	0.54
2:H:119:PHE:HB2	2:H:184:LEU:HD23	1.89	0.54
1:C:325:ALA:HB2	1:C:411:THR:HG21	1.90	0.54
1:E:287:ASN:O	1:E:380:MET:HE3	2.08	0.54
2:F:97:ASN:ND2	2:F:125:ASP:OD2	2.31	0.54
2:N:236:PRO:HG2	2:N:239:GLY:H	1.71	0.54
1:C:264:HIS:HE1	1:C:574:HIS:CD2	2.26	0.54
1:E:474:PRO:O	1:E:586:ARG:NH1	2.41	0.54
1:A:395:ASP:OD1	1:A:465:THR:HG23	2.07	0.54
1:G:149:THR:OG1	1:G:150:ASP:N	2.40	0.54
2:L:260:ASP:OD2	2:L:262:THR:OG1	2.26	0.54
1:M:53:HIS:CE1	1:M:139:TYR:HA	2.41	0.54
1:E:118:TRP:CD1	1:E:514:THR:HB	2.42	0.53
2:F:236:PRO:HG2	2:F:239:GLY:H	1.73	0.53
1:I:185:PHE:CG	1:I:186:GLN:N	2.76	0.53
1:O:253:GLN:NE2	1:O:608:GLU:OE2	2.39	0.53
1:C:185:PHE:CG	1:C:186:GLN:N	2.76	0.53
1:E:143:ARG:HE	1:E:177:PRO:HB3	1.73	0.53
1:G:479:GLU:OE1	1:G:586:ARG:NH1	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:375:PRO:HG2	1:M:376:HIS:CE1	2.43	0.53
1:E:446:THR:HG23	1:E:451:GLN:HB3	1.91	0.53
1:K:55:VAL:HG11	1:K:185:PHE:HA	1.89	0.53
1:A:201:PHE:HB3	1:A:230:ALA:HB3	1.90	0.53
1:G:239:ALA:HB3	1:G:270:ILE:HD12	1.90	0.53
2:J:106:ILE:HG22	2:J:107:LEU:HD12	1.89	0.53
1:I:309:SER:HB2	1:I:641:ALA:HB2	1.90	0.53
1:M:192:LEU:HA	1:M:195:LEU:HD13	1.91	0.53
2:N:95:TYR:CD2	2:N:128:LEU:HD21	2.43	0.53
2:D:181:TYR:CE1	2:D:194:ARG:HB3	2.43	0.53
1:A:242:ARG:NH2	1:A:615:TRP:HB3	2.24	0.53
2:F:206:ILE:HD13	2:F:228:LEU:HD23	1.89	0.53
1:M:380:MET:CE	1:M:387:SER:HB3	2.38	0.53
2:N:135:ASN:OD1	2:N:138:HIS:N	2.41	0.53
1:O:64:TYR:HA	1:O:67:ARG:HG2	1.90	0.53
2:P:167:TYR:CE2	2:P:181:TYR:HE2	2.26	0.53
1:A:363:ARG:HE	1:A:365:ASN:HD21	1.56	0.53
1:M:55:VAL:HG11	1:M:185:PHE:HA	1.91	0.53
1:E:355:LYS:HA	1:E:361:PRO:HA	1.90	0.53
2:P:167:TYR:CE2	2:P:181:TYR:CE2	2.96	0.53
1:A:606:LEU:HD12	1:A:609:LEU:HD12	1.91	0.53
2:D:77:ASN:ND2	2:D:99:ALA:HB2	2.24	0.53
2:D:115:LYS:HB2	2:D:179:ARG:HG2	1.90	0.53
1:M:275:ALA:HA	1:M:279:ALA:HA	1.91	0.53
1:A:64:TYR:CD1	1:A:67:ARG:HD2	2.45	0.52
2:F:74:ILE:O	2:F:252:ASN:ND2	2.41	0.52
1:G:262:LEU:HD11	1:G:286:MET:HE2	1.91	0.52
2:L:92:GLN:HG2	2:L:105:LYS:HD2	1.91	0.52
1:A:146:ASP:HA	1:A:173:LYS:NZ	2.24	0.52
1:C:294:ASN:OD1	1:C:313:ARG:NH2	2.42	0.52
1:C:377:ASP:OD2	1:C:574:HIS:ND1	2.42	0.52
2:F:176:GLY:HA2	2:F:179:ARG:HH11	1.73	0.52
1:K:62:TYR:HD2	1:K:137:ARG:HD3	1.74	0.52
1:M:53:HIS:HE1	1:M:140:TRP:H	1.56	0.52
1:C:89:ASN:HD22	2:D:205:VAL:HG21	1.75	0.52
1:C:210:VAL:HG13	1:C:454:THR:HG23	1.92	0.52
1:I:404:LEU:HA	1:I:407:GLN:HB2	1.91	0.52
1:I:210:VAL:HG21	1:I:454:THR:HG23	1.91	0.52
1:I:396:THR:OG1	1:I:398:ASP:OD1	2.20	0.52
1:K:69:LEU:O	1:K:73:LEU:HD12	2.09	0.52
2:P:78:ARG:NH1	2:P:122:SER:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:CG	1:A:186:GLN:N	2.78	0.52
2:D:93:THR:HB	2:D:107:LEU:HB2	1.92	0.52
2:J:68:PRO:HB3	2:J:83:GLU:HG2	1.91	0.52
1:K:198:LYS:HA	1:K:234:HIS:NE2	2.24	0.52
2:L:104:VAL:HG21	2:L:159:GLY:HA3	1.92	0.52
1:O:215:SER:HB3	1:O:572:THR:HG21	1.91	0.52
1:A:317:PHE:O	1:A:321:VAL:HG23	2.10	0.52
1:I:211:PRO:O	1:I:213:PRO:HD3	2.10	0.52
1:O:143:ARG:HD3	1:O:621:TYR:O	2.10	0.52
1:C:45:LEU:HB2	1:C:601:TRP:CD1	2.44	0.52
1:E:77:LEU:HD21	1:E:594:ILE:HD12	1.91	0.52
1:I:64:TYR:HE2	1:I:581:GLU:HB3	1.75	0.52
1:M:66:GLU:HG2	1:M:87:GLU:HB2	1.92	0.52
1:O:290:TYR:OH	1:O:313:ARG:O	2.19	0.52
1:C:376:HIS:CE1	1:C:419:ARG:HB3	2.45	0.51
1:G:557:GLN:HG2	1:G:560:MET:H	1.75	0.51
1:I:60:GLU:HG2	2:J:146:LYS:HG2	1.91	0.51
1:M:246:LEU:O	1:M:250:ILE:HG13	2.10	0.51
1:M:262:LEU:HD21	1:M:584:MET:HE1	1.91	0.51
1:M:377:ASP:HB3	1:M:380:MET:HB3	1.91	0.51
1:C:356:THR:HG22	1:C:357:HIS:N	2.25	0.51
1:E:195:LEU:HD22	1:E:236:TYR:HB3	1.92	0.51
1:I:632:ILE:HD12	1:I:632:ILE:H	1.75	0.51
1:K:275:ALA:HA	1:K:279:ALA:HA	1.92	0.51
1:M:572:THR:O	1:M:574:HIS:N	2.41	0.51
1:I:432:HIS:ND1	1:I:436:LEU:HA	2.26	0.51
1:A:508:THR:OG1	2:B:151:ALA:HB3	2.11	0.51
1:A:564:VAL:C	1:A:566:THR:H	2.19	0.51
1:C:67:ARG:HH12	2:D:194:ARG:NH2	2.09	0.51
1:C:584:MET:HA	1:C:588:VAL:HB	1.92	0.51
1:C:647:ARG:O	1:C:648:LYS:C	2.53	0.51
2:P:184:LEU:HG	2:P:186:MET:HE3	1.92	0.51
2:B:204:PRO:HG2	2:B:243:ILE:HD12	1.92	0.51
1:G:572:THR:OG1	2:H:145:ASN:OD1	2.27	0.51
1:C:185:PHE:O	1:C:187:ASN:N	2.44	0.51
1:E:321:VAL:HG11	1:E:408:ALA:HB1	1.91	0.51
1:E:475:LEU:HD23	1:E:480:LEU:HD21	1.92	0.51
1:M:216:THR:HA	1:M:569:GLN:OE1	2.11	0.51
1:O:211:PRO:O	1:O:384:PRO:HG2	2.11	0.51
1:O:487:TYR:CD2	1:O:490:ASP:HB3	2.46	0.51
1:A:559:GLU:O	1:A:563:GLU:N	2.37	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:VAL:N	1:C:281:ASP:OD2	2.41	0.51
1:I:242:ARG:NH2	1:I:615:TRP:HB3	2.26	0.51
1:K:256:GLU:OE2	1:K:345:SER:OG	2.25	0.51
1:K:500:ALA:HB3	1:K:503:GLN:HG3	1.92	0.51
1:M:375:PRO:HA	1:M:390:TRP:CD1	2.46	0.51
2:P:190:PHE:HE1	2:P:219:VAL:HG21	1.76	0.51
1:A:328:LYS:HA	1:A:366:HIS:HB3	1.93	0.51
2:J:148:CYS:HB2	2:J:174:PRO:HG3	1.93	0.51
1:K:316:THR:HG23	1:K:636:ILE:HA	1.93	0.51
1:M:138:PHE:HA	1:M:613:ALA:HB1	1.92	0.51
1:A:376:HIS:CE1	1:A:419:ARG:HG2	2.46	0.51
2:D:78:ARG:NH2	2:D:122:SER:O	2.44	0.51
2:N:72:PHE:HB3	2:N:80:PHE:HB2	1.92	0.51
1:A:76:ARG:HG3	1:A:590:TYR:CD2	2.46	0.50
1:C:56:ASN:C	1:C:56:ASN:HD22	2.17	0.50
1:I:77:LEU:HD21	1:I:594:ILE:HD13	1.94	0.50
2:J:100:LYS:HD2	2:J:102:ILE:HD11	1.92	0.50
1:K:66:GLU:OE2	1:K:133:SER:OG	2.24	0.50
1:M:571:PRO:HB3	2:N:143:GLY:HA3	1.92	0.50
1:C:68:SER:HB2	1:C:584:MET:HB2	1.92	0.50
2:D:68:PRO:HB3	2:D:83:GLU:HG2	1.92	0.50
2:D:148:CYS:HB2	2:D:174:PRO:HG3	1.93	0.50
1:M:186:GLN:C	1:M:188:GLY:H	2.20	0.50
1:O:372:TYR:CD1	1:O:415:ARG:HB2	2.46	0.50
1:C:155:PRO:HG3	1:C:519:TYR:CZ	2.46	0.50
1:C:372:TYR:CD1	1:C:415:ARG:HB2	2.46	0.50
1:E:185:PHE:CD1	1:E:214:PHE:HB2	2.44	0.50
1:A:368:THR:OG1	1:A:370:TRP:NE1	2.43	0.50
1:C:147:ASN:O	1:C:149:THR:N	2.44	0.50
2:F:68:PRO:HB3	2:F:83:GLU:HG2	1.94	0.50
2:F:139:ALA:HB3	2:F:142:MET:HG2	1.93	0.50
2:F:176:GLY:HA2	2:F:179:ARG:NH1	2.26	0.50
1:G:185:PHE:CG	1:G:186:GLN:N	2.79	0.50
1:A:516:TYR:CZ	1:A:520:ILE:HD13	2.47	0.50
1:C:85:LEU:HD23	1:C:134:PRO:HD3	1.93	0.50
2:F:104:VAL:HG21	2:F:159:GLY:HA3	1.94	0.50
1:I:378:ARG:NH2	1:I:444:ASP:OD1	2.45	0.50
1:K:317:PHE:HE2	1:K:412:LEU:HD11	1.77	0.50
1:K:445:SER:OG	1:K:486:ASP:OD2	2.27	0.50
1:C:138:PHE:HA	1:C:613:ALA:HB1	1.93	0.50
1:C:243:LEU:O	1:C:247:ILE:HG13	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLU:CD	2:F:146:LYS:HA	2.36	0.50
1:M:45:LEU:HD22	1:M:134:PRO:HB3	1.94	0.50
1:O:241:GLY:O	1:O:245:LYS:HG2	2.11	0.50
1:A:138:PHE:HA	1:A:613:ALA:HB1	1.92	0.50
1:A:419:ARG:NH2	1:A:441:PRO:O	2.44	0.50
1:C:63:ASP:OD1	1:C:137:ARG:NH1	2.44	0.50
1:C:643:ASP:O	1:C:644:ALA:C	2.55	0.50
2:B:209:TRP:NE1	2:B:221:ARG:HG3	2.27	0.50
2:H:107:LEU:HG	2:H:109:ALA:H	1.77	0.50
2:H:121:LEU:HD21	2:H:248:PHE:HD2	1.75	0.50
1:K:264:HIS:HE1	1:K:574:HIS:CD2	2.29	0.50
2:P:203:SER:HA	2:P:240:PHE:HB2	1.93	0.50
1:M:191:GLN:HG3	1:M:193:VAL:HG12	1.93	0.50
2:N:96:ASN:OD1	2:N:103:HIS:ND1	2.45	0.50
2:P:157:ASP:OD2	2:P:161:ARG:N	2.43	0.50
1:E:383:SER:HA	1:E:386:ARG:HD2	1.94	0.50
2:F:86:THR:HG1	2:F:90:ASN:HD21	1.56	0.50
1:I:372:TYR:CD1	1:I:415:ARG:HB2	2.47	0.50
1:M:378:ARG:NH2	1:M:444:ASP:OD1	2.38	0.50
1:A:168:PRO:HG2	1:A:171:SER:HB3	1.94	0.49
1:A:185:PHE:HD2	1:A:214:PHE:HB2	1.75	0.49
1:C:289:PRO:CA	1:C:380:MET:HE1	2.38	0.49
1:C:487:TYR:CD2	1:C:490:ASP:HB3	2.47	0.49
2:F:87:HIS:HA	2:F:264:GLU:HG2	1.94	0.49
1:G:55:VAL:HA	1:G:182:GLY:O	2.11	0.49
2:J:73:ARG:O	2:J:254:VAL:HG11	2.12	0.49
1:M:45:LEU:HB2	1:M:601:TRP:CE3	2.47	0.49
2:P:67:PRO:O	2:P:85:TYR:OH	2.26	0.49
1:K:279:ALA:HB2	1:K:323:LYS:HG2	1.94	0.49
2:L:74:ILE:HB	2:L:78:ARG:HB2	1.94	0.49
2:N:74:ILE:HD13	2:N:120:TRP:CD1	2.46	0.49
1:O:378:ARG:HH22	1:O:443:TRP:HB3	1.77	0.49
1:C:173:LYS:O	1:C:173:LYS:HD3	2.12	0.49
1:E:262:LEU:HD12	1:E:284:PHE:HB2	1.93	0.49
1:I:195:LEU:HG	1:I:236:TYR:HB3	1.95	0.49
1:I:448:THR:HG23	1:I:451:GLN:H	1.76	0.49
1:K:246:LEU:O	1:K:250:ILE:HD12	2.13	0.49
1:A:143:ARG:NH1	1:A:624:SER:O	2.45	0.49
1:A:270:ILE:HD12	1:A:270:ILE:H	1.77	0.49
1:C:159:LYS:HG3	1:C:616:LEU:HD23	1.94	0.49
1:C:645:GLU:O	1:C:646:GLN:C	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:THR:HG22	1:E:432:HIS:CE1	2.47	0.49
2:J:108:ASP:OD1	2:J:162:ARG:NH2	2.45	0.49
1:G:316:THR:HG23	1:G:636:ILE:HA	1.95	0.49
2:H:210:ILE:HG12	2:H:222:SER:HB2	1.94	0.49
1:I:565:ARG:C	1:I:567:TYR:H	2.21	0.49
2:L:136:THR:HA	2:L:142:MET:HE3	1.93	0.49
1:M:290:TYR:O	1:M:387:SER:OG	2.28	0.49
1:O:282:ALA:HB2	1:O:593:PRO:HG3	1.93	0.49
2:L:121:LEU:HD11	2:L:248:PHE:HD2	1.76	0.49
2:P:69:GLN:HE21	2:P:82:LEU:HD23	1.77	0.49
1:A:605:GLY:O	1:A:609:LEU:HG	2.12	0.49
2:L:244:ASP:OD2	2:L:246:SER:OG	2.30	0.49
1:M:350:TRP:N	1:M:596:TYR:O	2.45	0.49
1:M:387:SER:OG	1:M:388:ILE:N	2.46	0.49
1:A:173:LYS:HG3	1:A:173:LYS:O	2.13	0.49
1:C:285:VAL:HG23	1:C:371:ILE:HA	1.95	0.49
1:E:380:MET:HE2	1:E:574:HIS:HE1	1.76	0.49
1:G:172:ARG:C	1:G:174:ALA:H	2.21	0.49
1:K:185:PHE:HD1	1:K:214:PHE:CD2	2.30	0.49
2:N:121:LEU:HD22	2:N:186:MET:HE1	1.94	0.49
1:A:594:ILE:CG2	1:A:598:TRP:HE1	2.26	0.49
1:C:291:ALA:O	1:C:313:ARG:NH1	2.40	0.49
2:B:152:VAL:HG21	2:B:190:PHE:CZ	2.47	0.49
1:I:191:GLN:HB3	1:I:313:ARG:NH1	2.28	0.49
1:M:264:HIS:HE1	1:M:574:HIS:CD2	2.31	0.49
1:O:69:LEU:HD21	1:O:592:LEU:HD11	1.95	0.49
1:A:53:HIS:HE1	1:A:182:GLY:HA2	1.77	0.48
1:A:56:ASN:HB2	1:A:180:TRP:HE1	1.77	0.48
1:I:254:HIS:HB3	1:I:257:ASP:OD2	2.13	0.48
1:K:572:THR:OG1	2:L:145:ASN:ND2	2.44	0.48
1:O:396:THR:OG1	1:O:398:ASP:OD1	2.31	0.48
1:K:186:GLN:C	1:K:188:GLY:H	2.21	0.48
1:K:425:GLY:C	1:K:470:GLN:HG3	2.38	0.48
2:L:182:ASP:OD2	2:L:195:TYR:OH	2.25	0.48
2:N:94:PHE:CD1	2:N:105:LYS:HA	2.48	0.48
1:C:444:ASP:HB2	1:C:486:ASP:OD2	2.13	0.48
1:E:560:MET:O	1:E:564:VAL:HG23	2.13	0.48
1:I:215:SER:HB3	1:I:572:THR:HG21	1.95	0.48
1:O:211:PRO:O	1:O:213:PRO:HD3	2.12	0.48
1:E:45:LEU:HD22	1:E:134:PRO:HB3	1.95	0.48
1:E:378:ARG:HD3	1:E:570:ARG:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:446:THR:HG23	1:G:451:GLN:HB3	1.94	0.48
1:O:246:LEU:O	1:O:250:ILE:HD12	2.12	0.48
1:G:444:ASP:OD1	1:G:444:ASP:N	2.46	0.48
2:H:69:GLN:NE2	2:H:85:TYR:OH	2.38	0.48
2:P:135:ASN:OD1	2:P:137:ARG:N	2.47	0.48
1:C:67:ARG:HH22	2:D:194:ARG:NH2	2.11	0.48
2:D:77:ASN:OD1	2:D:99:ALA:N	2.42	0.48
1:G:143:ARG:NH1	1:G:144:ALA:O	2.46	0.48
2:H:127:PHE:CD1	2:H:211:LEU:HD21	2.49	0.48
1:I:493:GLN:HE22	1:I:499:TYR:H	1.60	0.48
1:M:57:SER:OG	1:M:60:GLU:OE1	2.25	0.48
1:O:210:VAL:N	1:O:211:PRO:HD3	2.29	0.48
2:F:82:LEU:HG	2:F:85:TYR:CD2	2.48	0.48
1:M:446:THR:HG23	1:M:451:GLN:HB3	1.95	0.48
1:A:155:PRO:HB2	1:A:180:TRP:CZ3	2.49	0.48
1:A:275:ALA:HA	1:A:279:ALA:HA	1.96	0.48
1:G:118:TRP:CD1	1:G:514:THR:HG23	2.49	0.48
1:G:643:ASP:OD1	1:G:644:ALA:N	2.46	0.48
2:L:181:TYR:CZ	2:L:194:ARG:HB2	2.48	0.48
1:M:363:ARG:HE	1:M:469:PRO:HG2	1.79	0.48
2:N:120:TRP:CZ3	2:N:185:VAL:HG21	2.49	0.48
1:C:500:ALA:HB3	1:C:503:GLN:HG3	1.96	0.48
1:E:175:LYS:HA	1:E:176:GLY:HA2	1.58	0.48
1:G:211:PRO:O	1:G:384:PRO:HG2	2.14	0.48
1:M:280:PRO:O	1:M:327:ASN:ND2	2.46	0.48
1:O:185:PHE:O	1:O:186:GLN:C	2.57	0.48
1:O:479:GLU:OE1	1:O:586:ARG:NH2	2.46	0.48
1:K:163:ASN:HD22	1:K:518:TYR:HA	1.79	0.47
1:M:264:HIS:HD2	1:M:578:PRO:HG3	1.78	0.47
1:O:138:PHE:HA	1:O:613:ALA:HB1	1.96	0.47
1:O:321:VAL:HG22	1:O:369:THR:HG21	1.95	0.47
1:C:51:PHE:HB3	1:C:62:TYR:CE1	2.49	0.47
1:C:376:HIS:CE1	1:C:484:ASP:HB2	2.47	0.47
2:F:133:THR:HA	2:F:150:ASN:OD1	2.14	0.47
1:G:195:LEU:HD22	1:G:236:TYR:HB3	1.96	0.47
1:M:294:ASN:OD1	1:M:313:ARG:NH2	2.47	0.47
1:A:66:GLU:HG3	1:A:135:VAL:HG21	1.97	0.47
1:C:245:LYS:O	1:C:249:THR:HG23	2.13	0.47
1:C:589:ALA:HA	1:C:592:LEU:HD23	1.96	0.47
2:B:93:THR:OG1	2:B:107:LEU:HB2	2.14	0.47
1:G:606:LEU:O	1:G:610:ARG:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:PRO:HG3	1:K:519:TYR:CE1	2.49	0.47
1:K:421:THR:HG22	1:K:432:HIS:CE1	2.49	0.47
1:M:60:GLU:HG3	2:N:146:LYS:HA	1.96	0.47
2:P:117:ARG:HD3	2:P:119:PHE:CZ	2.50	0.47
1:E:620:ASP:OD1	1:E:624:SER:OG	2.32	0.47
2:D:132:ALA:HB2	2:D:153:ILE:HG12	1.95	0.47
1:K:417:LEU:HD12	1:K:480:LEU:HD21	1.96	0.47
1:O:383:SER:OG	1:O:384:PRO:HD3	2.15	0.47
1:A:372:TYR:HD1	1:A:415:ARG:HB2	1.80	0.47
1:C:633:PRO:HD2	1:C:636:ILE:HD12	1.95	0.47
2:D:87:HIS:HA	2:D:264:GLU:HG2	1.97	0.47
1:K:393:LEU:HD21	1:K:404:LEU:HD23	1.96	0.47
1:K:429:ALA:O	1:K:465:THR:HA	2.15	0.47
1:M:211:PRO:O	1:M:384:PRO:HG2	2.14	0.47
1:M:212:LEU:HD11	1:M:302:TYR:CE1	2.49	0.47
1:M:243:LEU:O	1:M:247:ILE:HD12	2.15	0.47
1:M:558:GLU:O	1:M:560:MET:N	2.47	0.47
1:O:375:PRO:HG3	1:O:416:ILE:HD11	1.97	0.47
1:E:67:ARG:HG3	1:E:87:GLU:HG2	1.95	0.47
2:F:182:ASP:HB2	2:F:193:LEU:HB2	1.97	0.47
1:K:258:THR:CG2	1:K:331:LEU:HD13	2.43	0.47
1:K:515:ASP:HB3	1:K:519:TYR:CD2	2.49	0.47
1:A:64:TYR:HE2	2:B:171:THR:HG1	1.62	0.47
1:G:138:PHE:HA	1:G:613:ALA:HB1	1.95	0.47
1:G:211:PRO:HB2	1:G:213:PRO:HD3	1.95	0.47
1:G:214:PHE:HB2	1:G:379:VAL:HG22	1.96	0.47
1:G:279:ALA:HB2	1:G:323:LYS:HG2	1.97	0.47
1:G:350:TRP:HZ2	1:G:362:GLU:HG2	1.79	0.47
1:G:379:VAL:O	1:G:385:LEU:HD12	2.13	0.47
1:G:404:LEU:HA	1:G:407:GLN:HB2	1.97	0.47
1:I:77:LEU:HD22	1:I:598:TRP:HH2	1.80	0.47
1:I:557:GLN:C	1:I:559:GLU:H	2.22	0.47
1:M:444:ASP:OD1	1:M:444:ASP:N	2.47	0.47
1:A:246:LEU:O	1:A:250:ILE:HG12	2.15	0.47
1:C:57:SER:OG	1:C:60:GLU:OE1	2.32	0.47
1:C:372:TYR:HD1	1:C:415:ARG:HB2	1.80	0.47
1:E:201:PHE:H	1:E:230:ALA:HB3	1.79	0.47
2:F:184:LEU:HB2	2:F:191:TYR:HB2	1.96	0.47
1:K:192:LEU:HD23	1:K:290:TYR:HE2	1.80	0.47
1:K:515:ASP:HB3	1:K:519:TYR:HD2	1.79	0.47
1:M:290:TYR:OH	1:M:313:ARG:O	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:175:LYS:HA	1:O:176:GLY:HA2	1.55	0.47
1:O:325:ALA:HA	1:O:367:GLY:HA3	1.97	0.47
1:O:446:THR:HG22	1:O:452:ARG:HD2	1.97	0.47
1:C:564:VAL:HG12	1:C:564:VAL:O	2.15	0.47
1:C:572:THR:O	1:C:574:HIS:N	2.48	0.47
1:I:173:LYS:H	1:I:178:TRP:HE1	1.63	0.47
1:K:51:PHE:O	1:K:138:PHE:HB3	2.14	0.47
1:K:195:LEU:HD22	1:K:236:TYR:HB3	1.97	0.47
1:K:380:MET:HE3	1:K:574:HIS:HE1	1.80	0.47
1:K:416:ILE:HD12	1:K:464:LEU:HD12	1.97	0.47
2:N:69:GLN:OE1	2:N:85:TYR:OH	2.24	0.47
1:O:175:LYS:HD2	1:O:176:GLY:HA2	1.97	0.47
2:B:142:MET:HE1	2:B:172:GLN:O	2.15	0.47
1:E:642:GLU:OE1	1:E:642:GLU:N	2.39	0.47
2:F:157:ASP:N	2:F:157:ASP:OD1	2.47	0.47
1:G:77:LEU:HD13	1:G:598:TRP:HH2	1.79	0.47
1:G:516:TYR:CE1	1:G:520:ILE:HD13	2.50	0.47
1:I:158:ASN:OD1	1:I:161:GLY:N	2.48	0.47
1:O:64:TYR:OH	2:P:177:ALA:HB2	2.15	0.47
1:O:572:THR:N	2:P:143:GLY:O	2.46	0.47
1:M:202:ASN:OD1	1:M:203:ASN:N	2.47	0.46
1:C:263:SER:OG	1:C:284:PHE:O	2.31	0.46
1:I:246:LEU:O	1:I:250:ILE:HD12	2.15	0.46
1:I:378:ARG:NH2	1:I:444:ASP:O	2.48	0.46
1:M:155:PRO:HG3	1:M:519:TYR:CE1	2.50	0.46
1:E:378:ARG:NH2	1:E:446:THR:OG1	2.49	0.46
2:D:117:ARG:HB2	2:D:182:ASP:OD1	2.16	0.46
2:J:100:LYS:HG3	2:J:102:ILE:HG13	1.98	0.46
2:J:157:ASP:OD2	2:J:161:ARG:N	2.47	0.46
1:M:55:VAL:HG23	1:M:266:GLN:HB2	1.98	0.46
1:O:54:GLY:HA3	1:O:265:SER:OG	2.16	0.46
1:C:268:THR:OG1	1:C:289:PRO:HD2	2.15	0.46
1:C:377:ASP:CG	1:C:574:HIS:HD1	2.24	0.46
1:E:41:PRO:N	1:E:42:PRO:HD2	2.31	0.46
1:I:118:TRP:O	1:I:517:ARG:NH2	2.28	0.46
1:M:515:ASP:HB3	1:M:519:TYR:CD2	2.51	0.46
2:B:196:ARG:NH2	2:B:203:SER:OG	2.48	0.46
2:F:64:VAL:HG23	2:F:265:PRO:HB2	1.98	0.46
2:F:78:ARG:NH1	2:F:122:SER:O	2.47	0.46
1:I:76:ARG:HB2	1:I:590:TYR:HE1	1.80	0.46
1:I:316:THR:HG22	1:I:636:ILE:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:487:TYR:CD2	1:I:490:ASP:HB3	2.51	0.46
2:P:257:MET:HE2	2:P:257:MET:HB3	1.83	0.46
1:A:51:PHE:CE1	1:A:262:LEU:HD23	2.51	0.46
2:H:211:LEU:HD23	2:H:219:VAL:HG12	1.97	0.46
1:M:589:ALA:HA	1:M:592:LEU:HD13	1.97	0.46
1:A:264:HIS:HE1	1:A:574:HIS:CD2	2.34	0.46
1:A:281:ASP:OD1	1:A:330:ARG:NH1	2.49	0.46
1:C:67:ARG:HH22	2:D:194:ARG:CZ	2.29	0.46
1:E:326:GLU:O	1:E:329:THR:HG23	2.16	0.46
1:G:608:GLU:OE2	1:G:611:ARG:NH2	2.49	0.46
2:J:107:LEU:HD21	2:J:132:ALA:HA	1.98	0.46
2:P:130:PHE:CG	2:P:131:PRO:HD2	2.51	0.46
2:P:176:GLY:HA2	2:P:179:ARG:HD2	1.98	0.46
1:A:69:LEU:HD21	1:A:592:LEU:HD11	1.98	0.46
1:A:260:THR:HG23	1:A:282:ALA:HB3	1.98	0.46
1:E:130:ASP:OD1	2:F:237:SER:OG	2.24	0.46
2:L:132:ALA:HB2	2:L:153:ILE:HG12	1.98	0.46
2:F:141:CYS:HB2	2:F:147:GLY:O	2.16	0.46
1:G:192:LEU:HD21	1:G:272:LEU:HB2	1.97	0.46
1:M:303:PRO:HD2	1:M:306:GLU:HB2	1.97	0.46
1:C:55:VAL:HG23	1:C:266:GLN:HG2	1.98	0.45
1:C:143:ARG:HD2	1:C:621:TYR:O	2.17	0.45
1:G:73:LEU:HA	1:G:76:ARG:HB3	1.99	0.45
1:I:155:PRO:HG3	1:I:519:TYR:CE1	2.51	0.45
1:I:493:GLN:NE2	1:I:499:TYR:H	2.13	0.45
1:O:168:PRO:HB2	1:O:170:GLU:OE1	2.17	0.45
1:O:493:GLN:HG3	1:O:500:ALA:HB2	1.98	0.45
1:A:198:LYS:HA	1:A:234:HIS:NE2	2.31	0.45
1:A:378:ARG:HH22	1:A:446:THR:HG1	1.59	0.45
1:E:201:PHE:CE2	1:E:227:LEU:HD22	2.50	0.45
1:I:130:ASP:OD2	1:I:610:ARG:NH1	2.49	0.45
1:I:179:PHE:CZ	1:I:616:LEU:HD11	2.50	0.45
1:M:155:PRO:HG3	1:M:519:TYR:HE1	1.81	0.45
1:I:286:MET:HE1	1:I:584:MET:HE1	1.97	0.45
1:M:633:PRO:HD2	1:M:636:ILE:HD13	1.98	0.45
1:A:269:MET:HE2	1:A:289:PRO:HG2	1.99	0.45
1:C:155:PRO:HB2	1:C:180:TRP:CZ3	2.51	0.45
1:I:444:ASP:OD1	1:I:444:ASP:N	2.45	0.45
1:K:172:ARG:C	1:K:174:ALA:H	2.24	0.45
1:M:201:PHE:HB3	1:M:230:ALA:HB3	1.97	0.45
1:M:393:LEU:HD12	1:M:402:HIS:CG	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:C	1:A:187:ASN:N	2.74	0.45
1:A:265:SER:OG	1:A:266:GLN:N	2.50	0.45
1:A:381:GLY:HA3	1:A:443:TRP:HH2	1.81	0.45
2:J:74:ILE:HB	2:J:78:ARG:HB2	1.99	0.45
2:L:142:MET:HE1	2:L:172:GLN:O	2.16	0.45
2:N:86:THR:HG22	2:N:90:ASN:HD21	1.82	0.45
1:O:275:ALA:HA	1:O:279:ALA:HA	1.97	0.45
1:O:380:MET:HE1	1:O:574:HIS:HE1	1.82	0.45
1:A:444:ASP:OD1	1:A:444:ASP:N	2.47	0.45
1:C:89:ASN:ND2	2:D:205:VAL:HG11	2.30	0.45
1:E:493:GLN:HG3	1:E:500:ALA:HB2	1.98	0.45
2:D:124:ARG:HH11	2:D:124:ARG:HG2	1.81	0.45
1:G:129:GLY:O	2:H:196:ARG:NH1	2.50	0.45
1:M:143:ARG:HE	1:M:177:PRO:HB3	1.80	0.45
2:N:204:PRO:HG2	2:N:243:ILE:HD12	1.98	0.45
1:O:142:TYR:HB2	1:O:235:TYR:CD2	2.51	0.45
1:A:372:TYR:CD1	1:A:415:ARG:HB2	2.52	0.45
1:E:597:CYS:O	1:E:598:TRP:HB2	2.15	0.45
1:I:76:ARG:HB2	1:I:590:TYR:CE1	2.52	0.45
1:I:321:VAL:HG11	1:I:408:ALA:HB1	1.98	0.45
1:M:410:ASP:OD1	1:M:410:ASP:N	2.46	0.45
1:O:558:GLU:C	1:O:560:MET:H	2.25	0.45
1:C:479:GLU:O	1:C:582:ARG:NH1	2.49	0.45
1:E:262:LEU:HD21	1:E:584:MET:HE1	1.98	0.45
1:M:160:LYS:HE3	1:M:160:LYS:HA	1.97	0.45
1:M:565:ARG:C	1:M:567:TYR:H	2.24	0.45
1:O:89:ASN:HD22	2:P:205:VAL:HG21	1.82	0.45
1:O:242:ARG:NH2	1:O:615:TRP:HB3	2.32	0.45
1:O:487:TYR:HE1	1:O:570:ARG:HA	1.81	0.45
1:C:117:LYS:HA	1:C:517:ARG:NH1	2.32	0.45
2:D:182:ASP:HB2	2:D:193:LEU:HB2	1.99	0.45
1:G:363:ARG:HH12	1:G:590:TYR:HB3	1.82	0.45
2:H:88:CYS:HB2	2:H:261:ARG:HE	1.82	0.45
1:O:187:ASN:C	1:O:233:ARG:HH21	2.25	0.45
1:O:264:HIS:HE1	1:O:574:HIS:NE2	2.15	0.45
1:A:386:ARG:HH21	1:A:390:TRP:HH2	1.65	0.45
1:C:648:LYS:O	1:C:649:ALA:C	2.59	0.45
1:E:593:PRO:O	1:E:595:GLY:N	2.41	0.45
1:I:265:SER:OG	1:I:266:GLN:N	2.49	0.45
1:I:375:PRO:HB3	1:I:433:PHE:CE1	2.52	0.45
2:L:131:PRO:HG3	2:L:183:MET:SD	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:279:ALA:HB2	1:M:323:LYS:HG2	1.98	0.45
1:C:328:LYS:HA	1:C:366:HIS:HB3	1.99	0.44
1:I:262:LEU:HD12	1:I:286:MET:CE	2.45	0.44
2:N:68:PRO:HA	2:N:82:LEU:O	2.17	0.44
1:O:251:ARG:NH2	1:O:327:ASN:OD1	2.41	0.44
1:O:364:ASP:OD1	1:O:366:HIS:ND1	2.50	0.44
2:P:107:LEU:HG	2:P:109:ALA:H	1.81	0.44
2:B:241:TYR:HA	2:B:242:LYS:HA	1.78	0.44
1:G:175:LYS:HA	1:G:176:GLY:HA2	1.56	0.44
1:I:172:ARG:C	1:I:174:ALA:H	2.26	0.44
1:K:54:GLY:HA2	1:K:267:GLY:H	1.82	0.44
1:K:251:ARG:NH1	1:K:279:ALA:O	2.27	0.44
1:M:210:VAL:HG12	1:M:210:VAL:O	2.17	0.44
1:M:264:HIS:HA	1:M:286:MET:HB2	1.99	0.44
1:O:73:LEU:HD11	1:O:592:LEU:HD12	1.98	0.44
1:O:371:ILE:HG23	1:O:414:VAL:HA	1.99	0.44
1:A:430:GLN:HB2	1:K:432:HIS:HB3	1.99	0.44
1:C:494:SER:OG	1:C:495:GLY:N	2.50	0.44
1:E:286:MET:HG2	1:E:577:LEU:HD22	1.98	0.44
1:E:378:ARG:O	1:E:455:TRP:NE1	2.37	0.44
2:H:113:LEU:HB3	2:H:175:THR:HG22	2.00	0.44
2:J:87:HIS:CE1	2:J:89:GLU:HB2	2.53	0.44
1:C:383:SER:OG	1:C:384:PRO:HD3	2.17	0.44
1:I:263:SER:OG	1:I:285:VAL:HA	2.17	0.44
2:L:96:ASN:HD21	2:L:103:HIS:HD2	1.63	0.44
2:P:112:TYR:CD2	2:P:259:CYS:HB3	2.53	0.44
1:A:67:ARG:HH21	2:B:194:ARG:NE	2.14	0.44
1:C:312:ALA:HB2	1:C:639:ASP:HB2	1.99	0.44
1:E:160:LYS:HA	1:E:160:LYS:HD3	1.66	0.44
2:F:148:CYS:HB2	2:F:174:PRO:HG3	1.99	0.44
1:G:75:GLN:OE1	1:G:590:TYR:OH	2.35	0.44
1:I:263:SER:OG	1:I:284:PHE:O	2.26	0.44
1:K:175:LYS:HA	1:K:176:GLY:HA2	1.52	0.44
1:O:143:ARG:HA	1:O:179:PHE:HA	1.99	0.44
1:O:187:ASN:ND2	1:O:235:TYR:OH	2.51	0.44
1:A:192:LEU:HD23	1:A:290:TYR:HE2	1.81	0.44
1:K:143:ARG:HG3	1:K:622:TYR:HA	2.00	0.44
2:L:215:ASP:OD1	2:L:216:SER:N	2.50	0.44
1:M:380:MET:HE3	1:M:385:LEU:HB3	2.00	0.44
1:O:376:HIS:HE1	1:O:419:ARG:H	1.66	0.44
2:J:184:LEU:HD11	2:J:228:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ILE:HG22	1:C:312:ALA:HB3	2.00	0.44
1:E:432:HIS:CE1	1:E:436:LEU:HA	2.53	0.44
1:I:181:GLY:C	1:I:183:GLY:H	2.25	0.44
1:K:51:PHE:HB3	1:K:62:TYR:CE1	2.53	0.44
1:M:363:ARG:HH12	1:M:590:TYR:HB3	1.83	0.44
1:M:431:THR:OG1	1:M:464:LEU:O	2.31	0.44
1:G:220:ASN:HB3	1:G:221:GLY:H	1.56	0.44
1:I:383:SER:N	1:I:384:PRO:HD2	2.33	0.44
1:K:378:ARG:NH2	1:K:446:THR:OG1	2.50	0.44
1:M:186:GLN:C	1:M:188:GLY:N	2.76	0.44
1:O:383:SER:HA	1:O:386:ARG:HG3	2.00	0.44
1:A:286:MET:SD	1:A:578:PRO:HB3	2.57	0.43
1:A:374:ASN:ND2	1:A:576:THR:OG1	2.51	0.43
1:C:172:ARG:C	1:C:174:ALA:H	2.26	0.43
1:C:390:TRP:HZ2	1:C:442:PHE:HE2	1.65	0.43
1:E:73:LEU:HD22	1:E:594:ILE:HD13	1.99	0.43
2:N:215:ASP:OD1	2:N:217:SER:OG	2.31	0.43
2:P:75:ASP:N	2:P:75:ASP:OD1	2.50	0.43
1:A:143:ARG:HD2	1:A:622:TYR:HA	2.01	0.43
1:A:391:GLN:O	1:A:464:LEU:HD11	2.17	0.43
1:A:419:ARG:HD3	1:A:484:ASP:HB3	2.00	0.43
1:C:55:VAL:HA	1:C:182:GLY:O	2.18	0.43
1:C:433:PHE:HB2	1:C:464:LEU:HD23	2.00	0.43
2:F:95:TYR:CD2	2:F:128:LEU:HD21	2.53	0.43
1:I:365:ASN:C	1:I:593:PRO:HB3	2.43	0.43
2:J:92:GLN:HG3	2:J:108:ASP:HA	2.00	0.43
1:M:264:HIS:CE1	1:M:574:HIS:CD2	3.06	0.43
2:N:73:ARG:HA	2:N:73:ARG:HD3	1.80	0.43
1:C:265:SER:OG	1:C:266:GLN:N	2.50	0.43
2:F:130:PHE:CZ	2:F:257:MET:HE1	2.52	0.43
2:H:95:TYR:O	2:H:103:HIS:HA	2.19	0.43
1:K:196:TRP:NE1	1:K:630:PRO:O	2.43	0.43
1:K:372:TYR:CD1	1:K:415:ARG:HB2	2.52	0.43
1:O:386:ARG:HE	1:O:390:TRP:HZ3	1.67	0.43
1:O:578:PRO:HA	1:O:584:MET:HE3	2.01	0.43
1:A:139:TYR:O	1:A:242:ARG:NH2	2.52	0.43
1:E:51:PHE:HB3	1:E:62:TYR:CE1	2.53	0.43
1:E:69:LEU:HD11	1:E:592:LEU:HD11	2.00	0.43
1:E:220:ASN:CG	1:E:221:GLY:H	2.26	0.43
1:E:378:ARG:HH22	1:E:443:TRP:HB3	1.83	0.43
1:G:214:PHE:C	1:G:215:SER:HG	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:TRP:CE3	2:H:185:VAL:HG21	2.53	0.43
2:L:204:PRO:HG2	2:L:243:ILE:HD12	2.00	0.43
2:P:204:PRO:HG2	2:P:243:ILE:HD12	2.00	0.43
1:A:372:TYR:HB3	1:A:577:LEU:HD11	2.01	0.43
1:E:391:GLN:O	1:E:464:LEU:HD11	2.19	0.43
1:G:363:ARG:HD2	1:G:365:ASN:HD21	1.82	0.43
2:J:196:ARG:NH2	2:J:238:THR:O	2.49	0.43
1:E:185:PHE:C	1:E:187:ASN:H	2.27	0.43
2:F:96:ASN:HA	2:F:102:ILE:O	2.18	0.43
1:K:201:PHE:HB3	1:K:230:ALA:HB3	2.00	0.43
1:M:289:PRO:HA	1:M:380:MET:CE	2.48	0.43
1:M:372:TYR:CD1	1:M:415:ARG:HB2	2.54	0.43
1:O:233:ARG:HA	1:O:235:TYR:CE1	2.53	0.43
1:A:376:HIS:CD2	1:A:484:ASP:HB2	2.54	0.43
1:C:146:ASP:HA	1:C:173:LYS:NZ	2.33	0.43
2:B:181:TYR:OH	2:B:194:ARG:HD2	2.19	0.43
2:F:93:THR:OG1	2:F:107:LEU:HB2	2.18	0.43
1:G:429:ALA:O	1:G:465:THR:HA	2.19	0.43
2:J:115:LYS:HB2	2:J:179:ARG:HG3	2.00	0.43
1:M:143:ARG:NH1	1:M:624:SER:O	2.52	0.43
1:M:163:ASN:HB3	1:M:166:ASP:HB2	2.00	0.43
2:N:75:ASP:OD1	2:N:78:ARG:N	2.46	0.43
1:O:380:MET:HE1	1:O:574:HIS:CE1	2.53	0.43
1:A:279:ALA:HB1	1:A:324:VAL:HG22	2.01	0.43
1:E:375:PRO:HA	1:E:390:TRP:CD1	2.53	0.43
2:D:78:ARG:HG2	2:D:97:ASN:HD22	1.84	0.43
2:D:178:THR:C	2:D:180:ASP:H	2.25	0.43
1:G:69:LEU:O	1:G:73:LEU:HG	2.19	0.43
1:M:516:TYR:CE1	1:M:520:ILE:HD13	2.53	0.43
1:O:505:ASN:N	1:O:510:LYS:O	2.44	0.43
1:C:201:PHE:HB3	1:C:230:ALA:HB3	2.00	0.43
1:K:143:ARG:HH21	1:K:177:PRO:HB3	1.83	0.43
1:K:163:ASN:ND2	1:K:518:TYR:HA	2.33	0.43
2:L:93:THR:HG21	2:L:130:PHE:CZ	2.54	0.43
1:A:572:THR:O	1:A:574:HIS:N	2.46	0.43
1:C:54:GLY:HA3	1:C:265:SER:OG	2.18	0.43
2:B:115:LYS:HB2	2:B:179:ARG:HG3	2.01	0.43
1:E:285:VAL:HG23	1:E:371:ILE:HA	2.01	0.43
1:E:383:SER:OG	1:E:384:PRO:HD3	2.18	0.43
2:D:230:ARG:O	2:D:232:GLY:N	2.51	0.43
2:H:188:ASP:OD1	2:H:188:ASP:N	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:215:SER:OG	2:L:145:ASN:OD1	2.23	0.43
1:M:189:CYS:HA	1:M:302:TYR:OH	2.18	0.43
2:N:87:HIS:HA	2:N:264:GLU:HG2	2.00	0.43
2:N:134:LEU:HD13	2:N:141:CYS:SG	2.59	0.43
1:A:89:ASN:OD1	2:B:205:VAL:HG11	2.19	0.42
1:E:74:ASN:HD21	1:E:85:LEU:HB2	1.84	0.42
1:G:380:MET:HB3	1:G:390:TRP:HB2	2.00	0.42
1:I:320:ILE:O	1:I:324:VAL:HG23	2.19	0.42
1:I:584:MET:HA	1:I:588:VAL:HB	2.01	0.42
1:K:287:ASN:ND2	1:K:377:ASP:OD2	2.38	0.42
1:O:286:MET:HE2	1:O:578:PRO:HG3	2.01	0.42
1:A:142:TYR:HB2	1:A:235:TYR:CD2	2.54	0.42
1:A:184:PRO:O	1:A:185:PHE:HB3	2.18	0.42
1:C:328:LYS:HG3	1:C:329:THR:HG23	2.01	0.42
1:C:442:PHE:CD2	1:C:458:PRO:HD3	2.54	0.42
1:K:383:SER:OG	1:K:384:PRO:HD3	2.18	0.42
1:A:66:GLU:OE1	1:A:137:ARG:NH2	2.43	0.42
1:A:444:ASP:HB3	1:A:484:ASP:OD2	2.19	0.42
1:E:316:THR:HG23	1:E:636:ILE:HA	2.01	0.42
1:G:521:SER:O	1:G:523:TYR:N	2.51	0.42
1:I:215:SER:CB	1:I:572:THR:HG21	2.49	0.42
1:I:375:PRO:HG3	1:I:416:ILE:HD11	2.01	0.42
2:J:254:VAL:HG13	2:J:254:VAL:O	2.20	0.42
1:K:125:ILE:HD12	1:K:125:ILE:H	1.85	0.42
1:K:51:PHE:CE1	1:K:262:LEU:HD23	2.55	0.42
1:K:291:ALA:O	1:K:313:ARG:NH1	2.52	0.42
1:K:386:ARG:HH21	1:K:390:TRP:HH2	1.67	0.42
1:O:49:ILE:O	1:O:136:ILE:N	2.46	0.42
1:O:376:HIS:CE1	1:O:419:ARG:H	2.37	0.42
1:O:575:SER:C	1:O:578:PRO:HD2	2.45	0.42
2:P:117:ARG:HA	2:P:255:MET:O	2.20	0.42
1:E:42:PRO:HB2	1:E:43:LEU:H	1.66	0.42
1:G:165:TYR:CZ	1:G:522:LEU:HD21	2.54	0.42
1:G:282:ALA:HB2	1:G:593:PRO:HG3	2.02	0.42
1:K:53:HIS:N	1:K:62:TYR:OH	2.52	0.42
2:L:96:ASN:HD21	2:L:103:HIS:CD2	2.37	0.42
2:L:174:PRO:O	2:L:178:THR:HG23	2.20	0.42
1:O:88:ASN:ND2	1:O:133:SER:HB3	2.35	0.42
1:A:187:ASN:HB3	1:A:236:TYR:OH	2.20	0.42
2:B:202:PHE:HB3	2:B:241:TYR:HE1	1.82	0.42
1:G:250:ILE:C	1:G:252:ASN:H	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:THR:O	1:G:272:LEU:HG	2.20	0.42
1:K:285:VAL:HG22	1:K:370:TRP:O	2.19	0.42
2:P:126:ASP:OD1	2:P:126:ASP:N	2.50	0.42
1:A:45:LEU:H	1:A:601:TRP:HD1	1.66	0.42
1:E:432:HIS:ND1	1:E:436:LEU:HA	2.34	0.42
2:J:206:ILE:HD11	2:J:243:ILE:HD13	2.01	0.42
1:M:564:VAL:C	1:M:566:THR:N	2.78	0.42
2:P:87:HIS:CE1	2:P:89:GLU:HB2	2.55	0.42
1:C:386:ARG:HH22	1:C:458:PRO:HA	1.83	0.42
2:D:267:GLN:NE2	2:D:268:PRO:O	2.52	0.42
1:G:210:VAL:HB	1:G:211:PRO:HD3	2.02	0.42
1:M:195:LEU:O	1:M:234:HIS:HA	2.19	0.42
1:M:242:ARG:O	1:M:245:LYS:HG3	2.19	0.42
2:N:61:PRO:N	2:N:62:PRO:HD2	2.35	0.42
2:P:167:TYR:CD2	2:P:181:TYR:HE2	2.38	0.42
2:P:217:SER:OG	2:P:218:GLY:N	2.52	0.42
2:P:244:ASP:OD1	2:P:245:LEU:N	2.53	0.42
1:A:186:GLN:H	1:A:186:GLN:NE2	2.18	0.42
1:C:68:SER:OG	1:C:581:GLU:HA	2.20	0.42
1:C:447:THR:O	1:C:452:ARG:NH1	2.52	0.42
1:I:55:VAL:O	1:I:57:SER:N	2.53	0.42
1:M:51:PHE:HB3	1:M:62:TYR:CE1	2.55	0.42
2:N:94:PHE:HD1	2:N:105:LYS:HA	1.85	0.42
1:O:410:ASP:OD1	1:O:410:ASP:N	2.50	0.42
1:O:567:TYR:CE2	1:O:569:GLN:HA	2.54	0.42
1:A:419:ARG:HA	1:A:480:LEU:O	2.20	0.42
1:E:152:TYR:CD2	1:E:231:PRO:HB3	2.55	0.42
2:F:148:CYS:CB	2:F:174:PRO:HG3	2.50	0.42
1:G:445:SER:OG	1:G:486:ASP:OD2	2.37	0.42
1:A:487:TYR:OH	1:A:570:ARG:HB2	2.20	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.95	0.41
1:E:141:GLY:HA2	1:E:182:GLY:H	1.84	0.41
1:E:251:ARG:NH2	1:E:279:ALA:O	2.53	0.41
2:F:93:THR:HG21	2:F:111:GLY:N	2.35	0.41
2:H:78:ARG:HH21	2:H:120:TRP:CD1	2.37	0.41
2:J:87:HIS:HA	2:J:264:GLU:HG2	2.02	0.41
2:J:212:SER:OG	2:J:214:GLU:HG3	2.20	0.41
1:K:53:HIS:NE2	1:K:139:TYR:HA	2.35	0.41
1:O:172:ARG:C	1:O:174:ALA:H	2.28	0.41
1:O:619:ASP:OD2	1:O:621:TYR:HB3	2.20	0.41
2:P:175:THR:O	2:P:179:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	2:B:194:ARG:HE	2.16	0.41
1:C:155:PRO:HG3	1:C:519:TYR:CE1	2.54	0.41
1:E:372:TYR:CD1	1:E:415:ARG:HB2	2.54	0.41
1:E:479:GLU:CD	1:E:586:ARG:HH22	2.28	0.41
2:F:203:SER:HA	2:F:240:PHE:HB2	2.01	0.41
2:L:71:ILE:HD11	2:L:93:THR:HG23	2.01	0.41
2:L:250:PRO:HB2	2:L:252:ASN:OD1	2.19	0.41
1:M:46:PRO:HA	1:M:598:TRP:CD1	2.56	0.41
2:N:65:TYR:HB3	2:N:84:ASN:HA	2.02	0.41
2:N:67:PRO:HA	2:N:68:PRO:HD2	1.91	0.41
2:N:203:SER:HA	2:N:240:PHE:HB2	2.01	0.41
1:A:286:MET:HB3	1:A:577:LEU:HD22	2.03	0.41
1:E:479:GLU:OE1	1:E:586:ARG:NH2	2.54	0.41
1:I:125:ILE:HD12	1:I:125:ILE:H	1.86	0.41
1:K:421:THR:HG22	1:K:432:HIS:NE2	2.36	0.41
1:M:289:PRO:HA	1:M:380:MET:HE2	2.02	0.41
1:M:588:VAL:O	1:M:591:ASP:N	2.52	0.41
1:O:195:LEU:HB3	1:O:237:ALA:HB2	2.01	0.41
1:O:317:PHE:O	1:O:321:VAL:HG23	2.21	0.41
1:G:290:TYR:C	1:G:387:SER:HB2	2.45	0.41
1:I:287:ASN:O	1:I:380:MET:HE3	2.20	0.41
1:A:159:LYS:HG3	1:A:616:LEU:HD23	2.02	0.41
1:A:500:ALA:O	1:A:501:TYR:C	2.63	0.41
1:I:49:ILE:N	1:I:134:PRO:O	2.44	0.41
1:A:127:LYS:O	2:B:226:TYR:OH	2.30	0.41
1:A:365:ASN:C	1:A:593:PRO:HB3	2.44	0.41
1:C:444:ASP:OD1	1:C:444:ASP:N	2.54	0.41
2:B:186:MET:HE3	2:B:186:MET:HB3	1.90	0.41
2:F:206:ILE:HD11	2:F:243:ILE:HD13	2.02	0.41
1:G:185:PHE:HE1	1:G:214:PHE:H	1.69	0.41
1:I:241:GLY:HA3	1:I:630:PRO:HG3	2.02	0.41
1:K:189:CYS:HA	1:K:302:TYR:OH	2.21	0.41
1:O:290:TYR:O	1:O:388:ILE:HG12	2.20	0.41
1:C:130:ASP:HB3	2:D:237:SER:HB3	2.01	0.41
1:E:215:SER:O	1:E:216:THR:C	2.64	0.41
2:L:112:TYR:HE2	2:L:261:ARG:HH21	1.69	0.41
1:I:192:LEU:HA	1:I:195:LEU:HD13	2.03	0.41
1:I:599:HIS:O	1:I:600:SER:C	2.64	0.41
1:K:54:GLY:HA2	1:K:267:GLY:N	2.35	0.41
1:K:179:PHE:CE2	1:K:616:LEU:HD11	2.56	0.41
1:O:371:ILE:HD11	1:O:388:ILE:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:396:THR:OG1	1:O:400:THR:OG1	2.30	0.41
1:A:55:VAL:HA	1:A:182:GLY:O	2.21	0.41
1:A:79:LEU:HB3	1:A:84:GLY:HA2	2.02	0.41
1:A:125:ILE:HD12	1:A:125:ILE:H	1.85	0.41
1:A:571:PRO:HB3	2:B:142:MET:O	2.21	0.41
1:C:288:SER:O	1:C:387:SER:OG	2.33	0.41
1:E:298:THR:HG23	1:E:302:TYR:CD2	2.56	0.41
1:G:185:PHE:CZ	1:G:217:GLN:HG3	2.55	0.41
1:G:372:TYR:CD1	1:G:415:ARG:HB2	2.56	0.41
1:G:378:ARG:HH22	1:G:443:TRP:HB3	1.86	0.41
2:H:89:GLU:HB3	2:H:113:LEU:HD21	2.03	0.41
2:H:156:THR:HG21	2:H:218:GLY:HA3	2.03	0.41
2:J:157:ASP:OD1	2:J:157:ASP:N	2.53	0.41
1:M:50:ILE:HG21	1:M:243:LEU:HD11	2.03	0.41
1:M:215:SER:O	1:M:216:THR:C	2.64	0.41
1:M:286:MET:HE2	1:M:577:LEU:HD23	2.03	0.41
1:M:382:SER:O	1:M:386:ARG:HG2	2.20	0.41
1:M:516:TYR:HE1	1:M:520:ILE:HD13	1.86	0.41
2:N:127:PHE:C	2:N:128:LEU:HD12	2.46	0.41
1:O:76:ARG:HH21	1:O:594:ILE:HD13	1.85	0.41
1:O:391:GLN:O	1:O:464:LEU:HD11	2.21	0.41
1:O:508:THR:HG22	2:P:132:ALA:HB1	2.02	0.41
2:P:85:TYR:HB3	2:P:91:GLY:HA3	2.03	0.41
1:A:502:GLY:HA3	1:A:516:TYR:CZ	2.56	0.41
2:D:196:ARG:NH2	2:D:238:THR:O	2.53	0.41
2:F:206:ILE:O	2:F:207:LEU:HD23	2.21	0.41
2:J:193:LEU:HG	2:J:206:ILE:HG12	2.03	0.41
1:K:424:GLY:O	1:K:471:VAL:HG22	2.21	0.41
1:K:514:THR:O	1:K:514:THR:OG1	2.38	0.41
1:K:584:MET:HA	1:K:588:VAL:HB	2.03	0.41
1:M:173:LYS:HD3	1:M:173:LYS:HA	1.76	0.41
1:O:368:THR:HA	1:O:411:THR:HB	2.03	0.41
2:H:64:VAL:HG23	2:H:267:GLN:HG3	2.02	0.40
1:I:258:THR:CG2	1:I:593:PRO:HG2	2.51	0.40
2:J:127:PHE:CD1	2:J:211:LEU:HD21	2.55	0.40
1:K:55:VAL:HG22	1:K:182:GLY:O	2.20	0.40
1:A:49:ILE:HD11	1:A:592:LEU:HD13	2.03	0.40
1:E:615:TRP:H	1:E:615:TRP:CD1	2.38	0.40
2:F:73:ARG:O	2:F:254:VAL:HG11	2.21	0.40
2:F:74:ILE:HD11	2:F:80:PHE:CE2	2.56	0.40
1:G:432:HIS:ND1	1:G:436:LEU:HA	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:97:ASN:HB3	2:J:102:ILE:HB	2.02	0.40
1:K:398:ASP:OD1	1:K:398:ASP:N	2.53	0.40
1:K:479:GLU:OE1	1:K:586:ARG:NH1	2.52	0.40
1:O:419:ARG:NH2	1:O:441:PRO:O	2.55	0.40
2:P:86:THR:OG1	2:P:90:ASN:ND2	2.43	0.40
1:A:559:GLU:O	1:A:560:MET:C	2.64	0.40
1:C:70:CYS:SG	1:C:133:SER:OG	2.73	0.40
1:I:377:ASP:OD2	1:I:574:HIS:ND1	2.55	0.40
2:J:117:ARG:HG2	2:J:255:MET:HB3	2.02	0.40
1:K:175:LYS:HD3	1:K:176:GLY:HA2	2.02	0.40
2:N:82:LEU:HD12	2:N:92:GLN:O	2.21	0.40
2:N:107:LEU:HD21	2:N:132:ALA:HA	2.03	0.40
1:O:62:TYR:HD2	1:O:137:ARG:HD3	1.87	0.40
1:O:139:TYR:O	1:O:242:ARG:NH2	2.55	0.40
2:P:83:GLU:OE2	2:P:103:HIS:NE2	2.41	0.40
1:A:471:VAL:HG11	1:A:587:VAL:HA	2.03	0.40
1:A:642:GLU:OE1	1:A:642:GLU:N	2.42	0.40
1:C:217:GLN:H	1:C:217:GLN:HG2	1.65	0.40
1:C:486:ASP:C	1:C:571:PRO:HG2	2.46	0.40
1:G:62:TYR:CD2	1:G:137:ARG:HG2	2.56	0.40
2:J:81:THR:OG1	2:J:94:PHE:HB2	2.22	0.40
1:K:192:LEU:HD12	1:K:273:ALA:HB2	2.03	0.40
1:K:386:ARG:NH2	1:K:458:PRO:HA	2.36	0.40
1:K:516:TYR:CE1	1:K:520:ILE:HD13	2.57	0.40
1:O:507:GLU:O	2:P:107:LEU:HD11	2.21	0.40
1:A:189:CYS:HA	1:A:302:TYR:OH	2.22	0.40
1:A:433:PHE:HB2	1:A:464:LEU:HD23	2.03	0.40
1:C:175:LYS:HA	1:C:176:GLY:HA2	1.59	0.40
1:C:317:PHE:HE1	1:C:412:LEU:HD11	1.86	0.40
1:E:215:SER:OG	2:F:145:ASN:ND2	2.55	0.40
1:E:595:GLY:O	1:E:596:TYR:C	2.65	0.40
1:I:175:LYS:HA	1:I:176:GLY:HA2	1.60	0.40
1:I:290:TYR:OH	1:I:313:ARG:O	2.34	0.40
1:K:55:VAL:CG1	1:K:185:PHE:HA	2.51	0.40
1:K:147:ASN:OD1	1:K:148:GLU:N	2.55	0.40
1:M:191:GLN:NE2	1:M:194:SER:OG	2.55	0.40
2:P:189:GLY:HA3	2:P:209:TRP:O	2.22	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	529/658 (80%)	475 (90%)	45 (8%)	9 (2%)	7	35
1	C	518/658 (79%)	463 (89%)	49 (10%)	6 (1%)	10	41
1	E	543/658 (82%)	481 (89%)	49 (9%)	13 (2%)	4	29
1	G	548/658 (83%)	480 (88%)	55 (10%)	13 (2%)	4	29
1	I	531/658 (81%)	473 (89%)	48 (9%)	10 (2%)	6	33
1	K	534/658 (81%)	493 (92%)	38 (7%)	3 (1%)	21	54
1	M	518/658 (79%)	472 (91%)	34 (7%)	12 (2%)	5	30
1	O	507/658 (77%)	464 (92%)	35 (7%)	8 (2%)	7	36
2	B	213/274 (78%)	193 (91%)	18 (8%)	2 (1%)	14	46
2	D	208/274 (76%)	191 (92%)	16 (8%)	1 (0%)	24	57
2	F	211/274 (77%)	197 (93%)	13 (6%)	1 (0%)	24	57
2	H	209/274 (76%)	192 (92%)	15 (7%)	2 (1%)	12	45
2	J	214/274 (78%)	191 (89%)	23 (11%)	0	100	100
2	L	204/274 (74%)	188 (92%)	15 (7%)	1 (0%)	24	57
2	N	204/274 (74%)	189 (93%)	15 (7%)	0	100	100
2	P	202/274 (74%)	180 (89%)	22 (11%)	0	100	100
All	All	5893/7456 (79%)	5322 (90%)	490 (8%)	81 (1%)	9	38

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PRO
1	A	211	PRO
1	A	501	TYR
1	A	560	MET
1	E	211	PRO
1	E	220	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	42	PRO
1	G	223	ARG
1	G	522	LEU
1	I	56	ASN
1	I	601	TRP
1	K	211	PRO
1	K	213	PRO
1	M	211	PRO
1	M	213	PRO
1	M	215	SER
1	O	643	ASP
1	A	185	PHE
1	C	211	PRO
2	B	240	PHE
1	E	216	THR
1	E	530	MET
1	E	557	GLN
1	E	573	ASP
1	E	596	TYR
1	G	56	ASN
1	G	227	LEU
1	G	573	ASP
1	I	185	PHE
1	I	211	PRO
1	I	557	GLN
1	I	573	ASP
1	I	600	SER
1	I	655	LEU
1	K	573	ASP
1	M	216	THR
1	M	558	GLU
1	M	559	GLU
1	M	562	GLU
1	O	213	PRO
1	O	218	VAL
1	O	573	ASP
1	A	216	THR
1	C	186	GLN
1	E	42	PRO
1	M	56	ASN
1	M	565	ARG
1	O	211	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	219	LEU
1	C	573	ASP
1	E	43	LEU
1	E	56	ASN
1	E	210	VAL
1	E	524	GLY
1	G	215	SER
1	G	220	ASN
1	G	226	LEU
1	I	599	HIS
1	M	573	ASP
1	A	186	GLN
1	C	187	ASN
1	C	213	PRO
1	E	594	ILE
2	F	225	ALA
1	G	211	PRO
1	G	521	SER
2	H	241	TYR
1	I	558	GLU
2	L	230	ARG
1	M	174	ALA
1	M	566	THR
1	O	217	GLN
1	C	148	GLU
2	D	230	ARG
2	H	234	GLU
1	O	568	VAL
1	A	255	PRO
1	A	46	PRO
1	G	46	PRO
1	G	213	PRO
2	B	230	ARG

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	402/559 (72%)	399 (99%)	3 (1%)	76	78
1	C	396/559 (71%)	396 (100%)	0	100	100
1	E	398/559 (71%)	398 (100%)	0	100	100
1	G	400/559 (72%)	399 (100%)	1 (0%)	86	83
1	I	393/559 (70%)	392 (100%)	1 (0%)	86	83
1	K	399/559 (71%)	398 (100%)	1 (0%)	86	83
1	M	392/559 (70%)	391 (100%)	1 (0%)	86	83
1	O	382/559 (68%)	382 (100%)	0	100	100
2	B	174/234 (74%)	174 (100%)	0	100	100
2	D	169/234 (72%)	169 (100%)	0	100	100
2	F	170/234 (73%)	170 (100%)	0	100	100
2	H	168/234 (72%)	168 (100%)	0	100	100
2	J	172/234 (74%)	172 (100%)	0	100	100
2	L	165/234 (70%)	165 (100%)	0	100	100
2	N	164/234 (70%)	164 (100%)	0	100	100
2	P	163/234 (70%)	163 (100%)	0	100	100
All	All	4507/6344 (71%)	4500 (100%)	7 (0%)	87	85

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

Mol	Chain	Res	Type
1	A	184	PRO
1	A	185	PHE
1	A	186	GLN
1	G	185	PHE
1	I	185	PHE
1	K	185	PHE
1	M	564	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	191	GLN
1	A	264	HIS
1	A	430	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	462	GLN
1	A	599	HIS
1	C	191	GLN
1	C	264	HIS
1	C	376	HIS
1	C	391	GLN
1	C	420	ASN
1	C	462	GLN
1	C	569	GLN
1	E	89	ASN
1	E	191	GLN
1	E	264	HIS
1	E	366	HIS
1	E	462	GLN
1	E	612	GLN
2	D	96	ASN
2	F	84	ASN
2	F	145	ASN
1	G	391	GLN
1	G	407	GLN
1	G	493	GLN
1	G	503	GLN
1	G	638	GLN
2	H	84	ASN
2	H	101	ASN
1	I	88	ASN
1	I	252	ASN
1	I	638	GLN
1	K	191	GLN
1	K	462	GLN
1	K	493	GLN
2	L	96	ASN
1	M	53	HIS
1	M	264	HIS
1	M	407	GLN
1	O	83	HIS
1	O	264	HIS
1	O	287	ASN
1	O	503	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 8 ligands modelled in this entry, 8 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	541/658 (82%)	-0.37	0 100 100	54, 89, 117, 138	0
1	C	530/658 (80%)	-0.37	2 (0%) 88 70	49, 83, 114, 142	0
1	E	553/658 (84%)	-0.31	1 (0%) 91 80	51, 95, 123, 143	0
1	G	558/658 (84%)	-0.32	0 100 100	49, 93, 125, 173	0
1	I	543/658 (82%)	-0.27	1 (0%) 91 80	49, 97, 126, 148	0
1	K	546/658 (82%)	-0.32	2 (0%) 88 70	53, 95, 129, 152	0
1	M	530/658 (80%)	-0.29	2 (0%) 88 70	75, 106, 140, 165	0
1	O	521/658 (79%)	-0.24	1 (0%) 91 80	83, 133, 169, 183	0
2	B	215/274 (78%)	-0.41	0 100 100	74, 93, 141, 172	0
2	D	210/274 (76%)	-0.44	0 100 100	64, 93, 124, 163	0
2	F	213/274 (77%)	-0.42	0 100 100	68, 97, 132, 155	0
2	H	211/274 (77%)	-0.39	0 100 100	77, 123, 145, 175	0
2	J	216/274 (78%)	-0.43	0 100 100	64, 95, 146, 191	0
2	L	206/274 (75%)	-0.28	1 (0%) 87 66	79, 115, 141, 156	0
2	N	206/274 (75%)	-0.33	1 (0%) 87 66	83, 129, 150, 161	0
2	P	204/274 (74%)	-0.16	0 100 100	117, 181, 204, 221	0
All	All	6003/7456 (80%)	-0.32	11 (0%) 91 80	49, 100, 155, 221	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	519	TYR	4.8
1	K	216	THR	3.3
1	M	515	ASP	3.0
1	M	141	GLY	2.6
1	E	212	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	129	ALA	2.4
1	I	193	VAL	2.4
1	C	217	GLN	2.3
1	K	136	ILE	2.3
2	L	132	ALA	2.3
1	C	282	ALA	2.2

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](#)

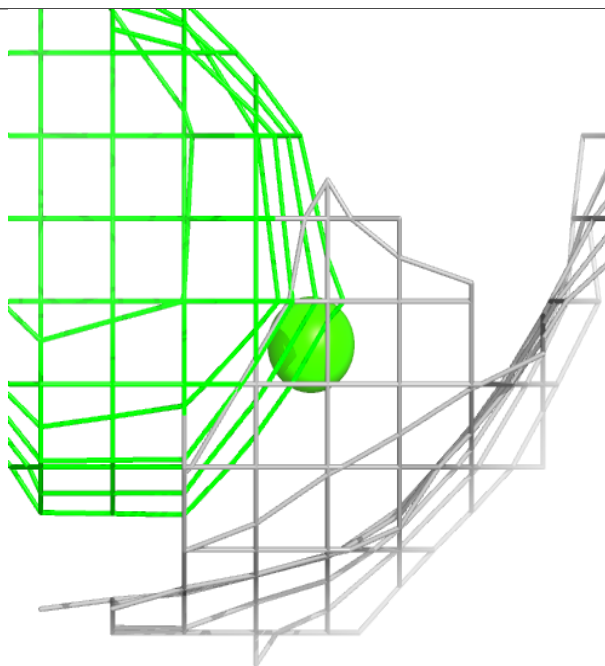
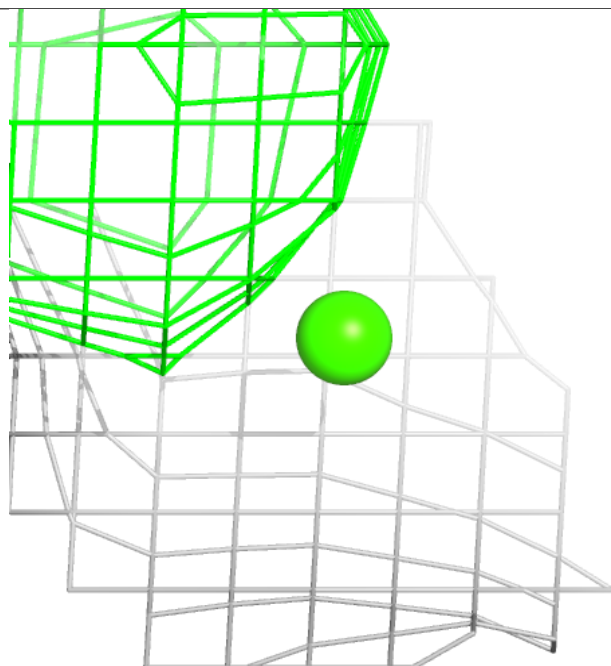
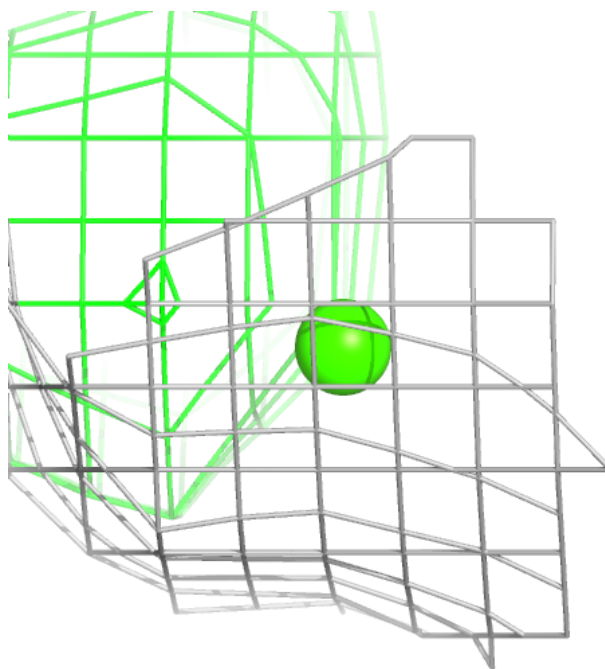
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	CA	A	701	1/1	0.95	0.09	83,83,83,83	0
3	CA	K	701	1/1	0.95	0.08	81,81,81,81	0
3	CA	O	701	1/1	0.95	0.11	106,106,106,106	0
3	CA	C	701	1/1	0.96	0.10	72,72,72,72	0
3	CA	M	701	1/1	0.96	0.12	91,91,91,91	0
3	CA	I	701	1/1	0.96	0.08	70,70,70,70	0
3	CA	G	701	1/1	0.97	0.04	83,83,83,83	0
3	CA	E	701	1/1	0.99	0.05	76,76,76,76	0

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

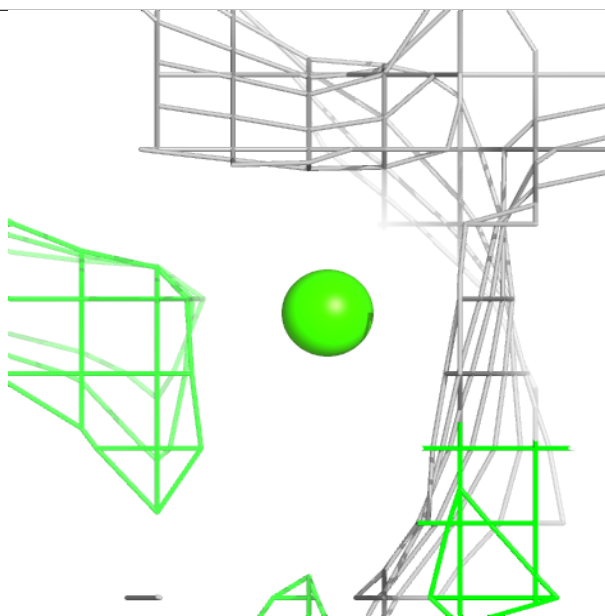
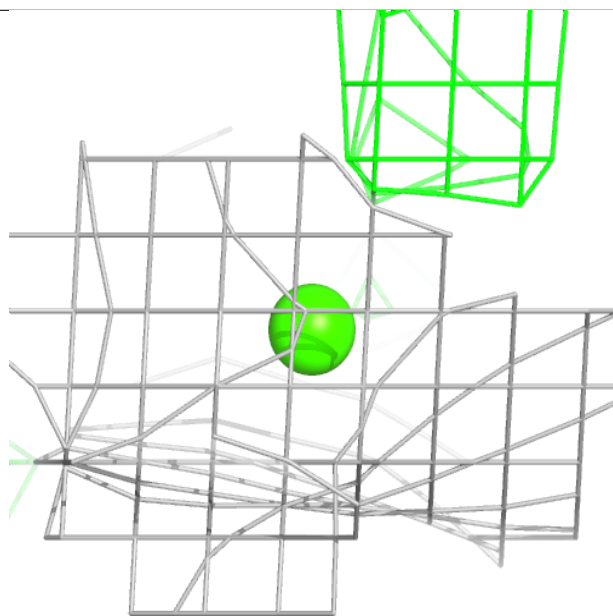
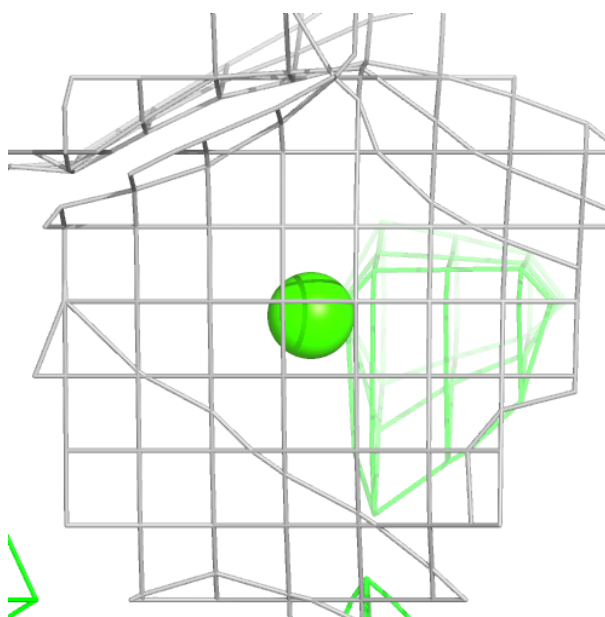
Electron density around CA A 701:

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



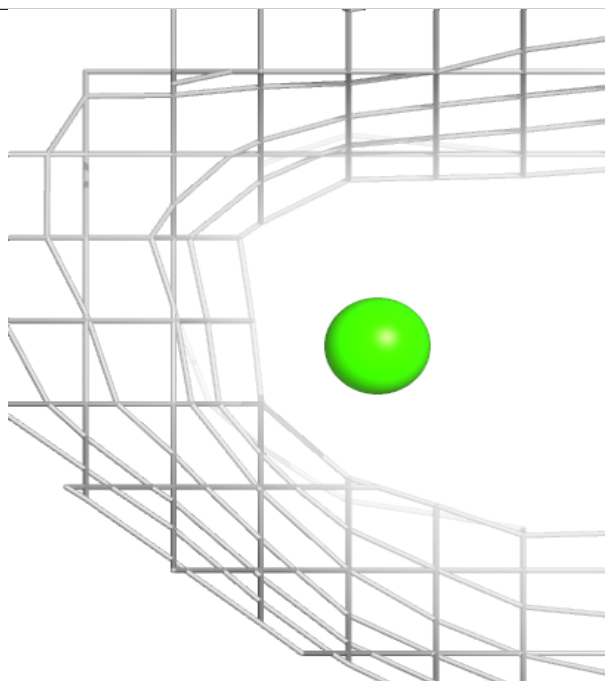
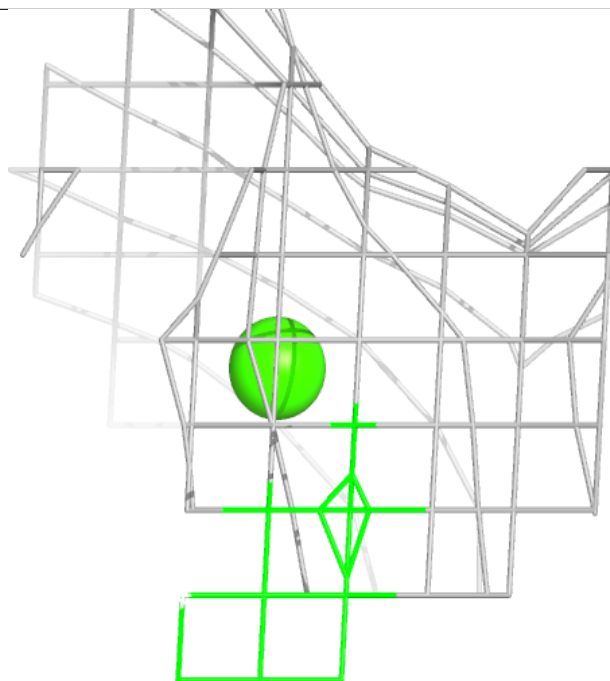
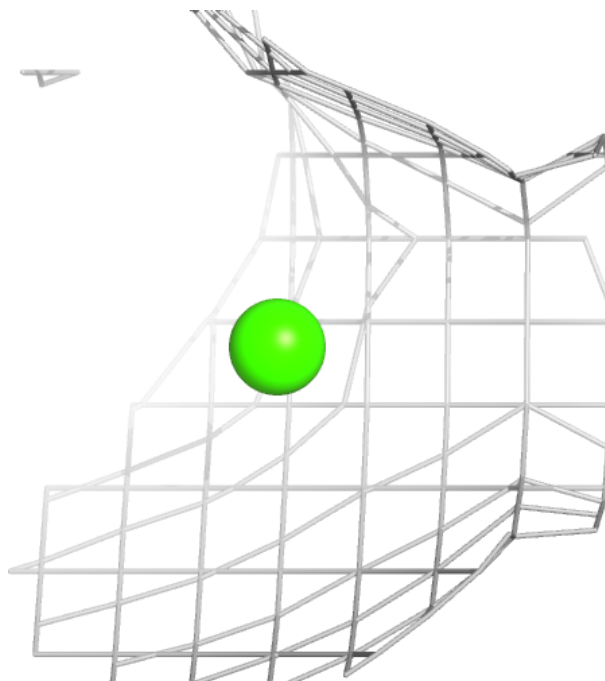
Electron density around CA K 701:

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



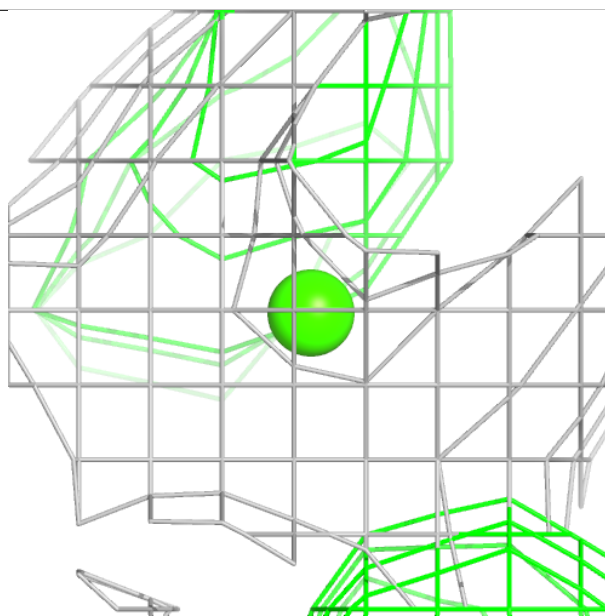
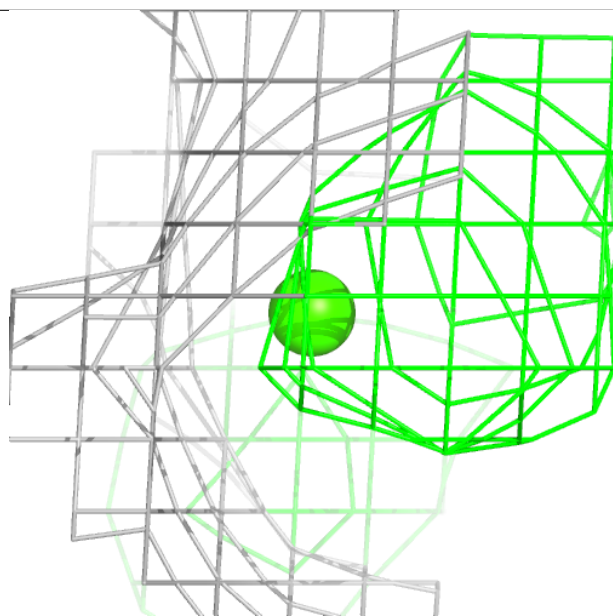
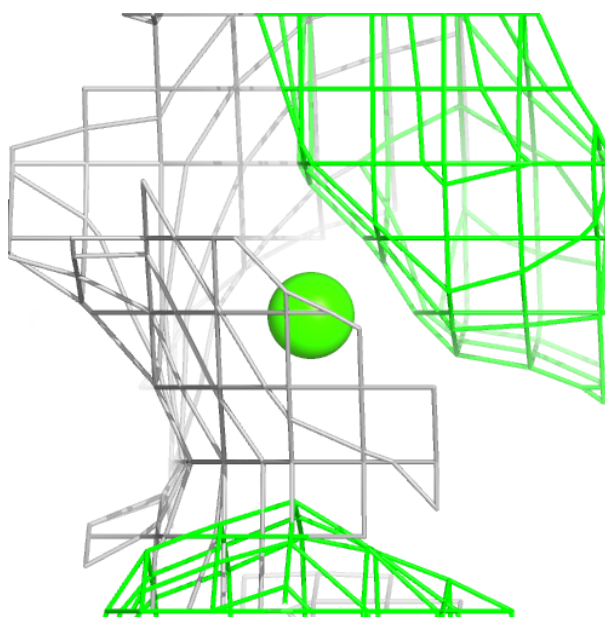
Electron density around CA O 701:

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



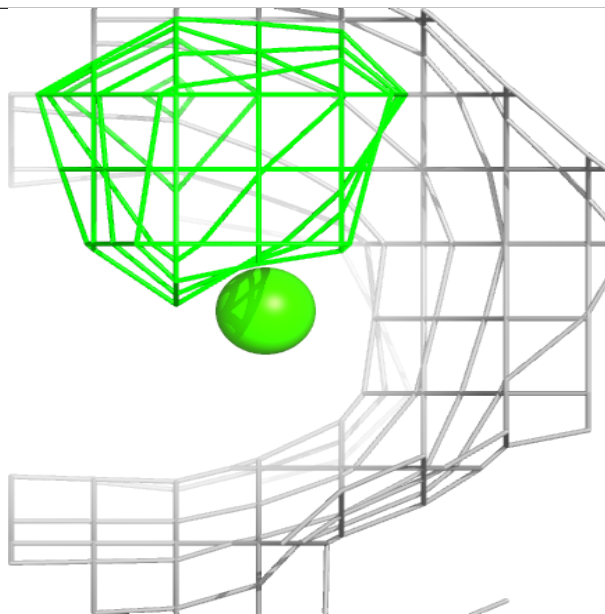
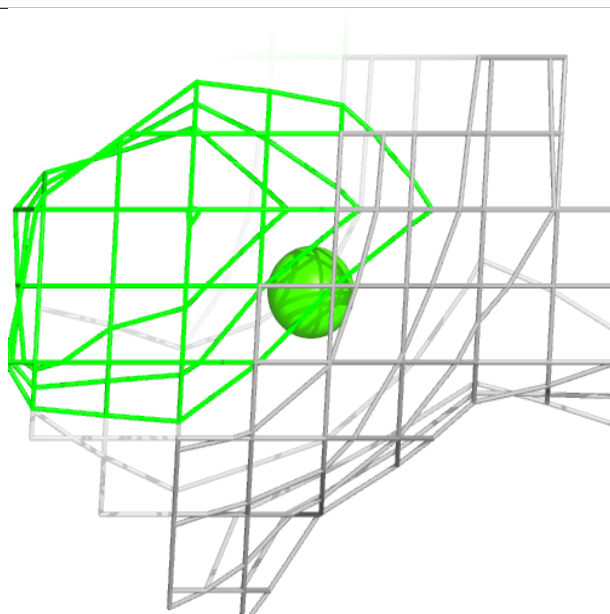
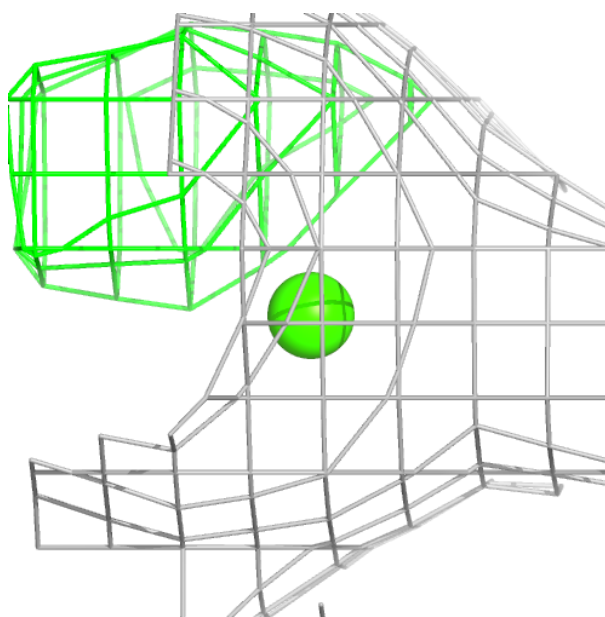
Electron density around CA C 701:

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



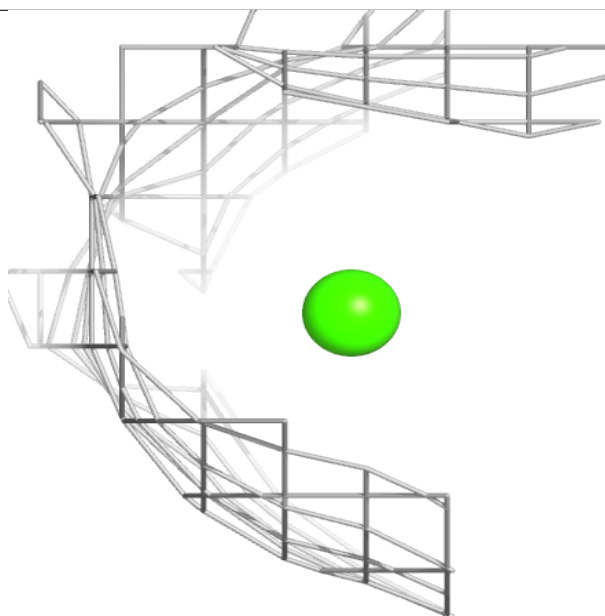
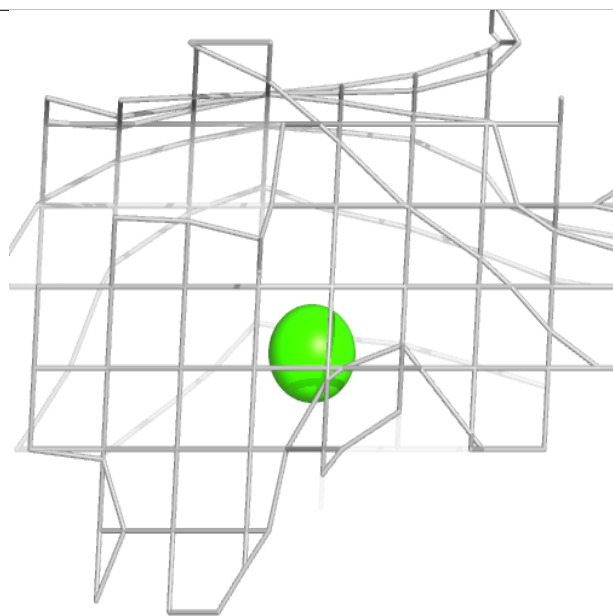
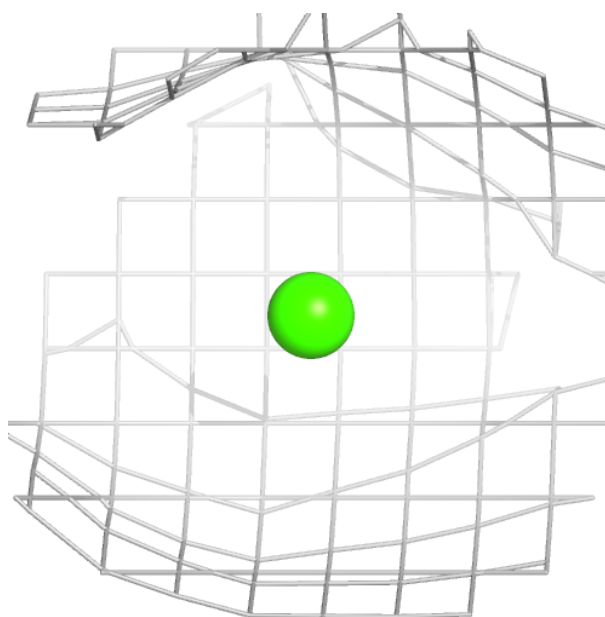
Electron density around CA M 701:

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



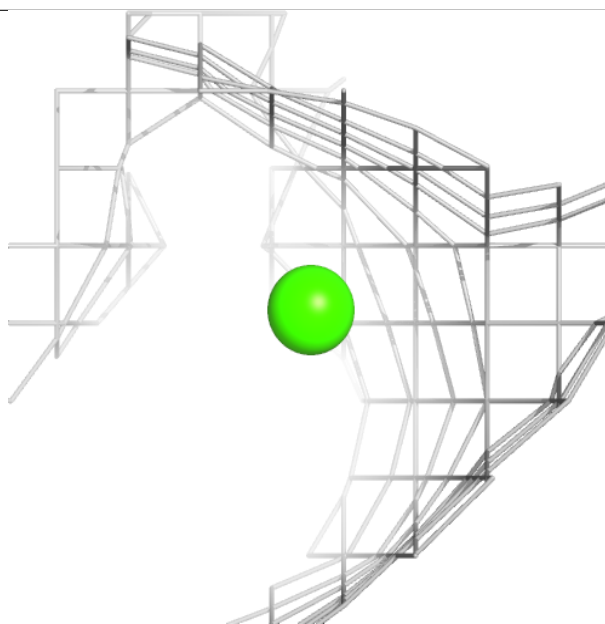
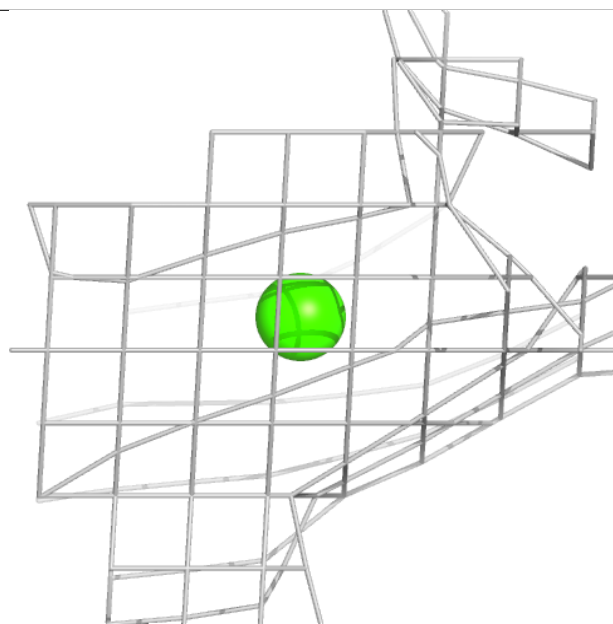
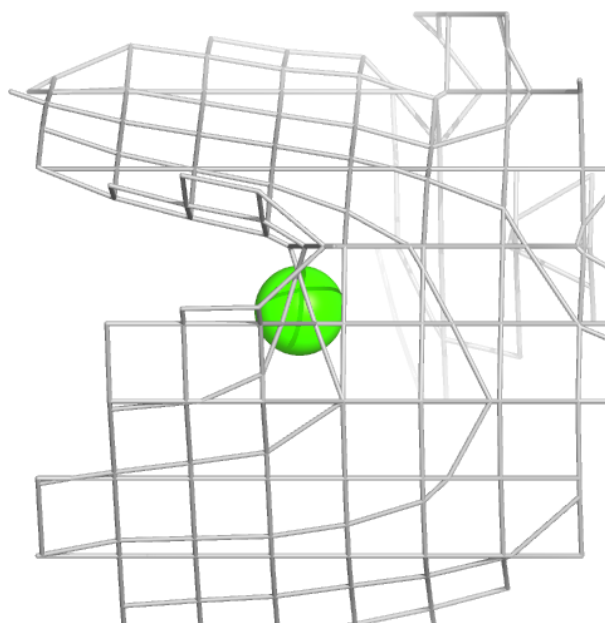
Electron density around CA I 701:

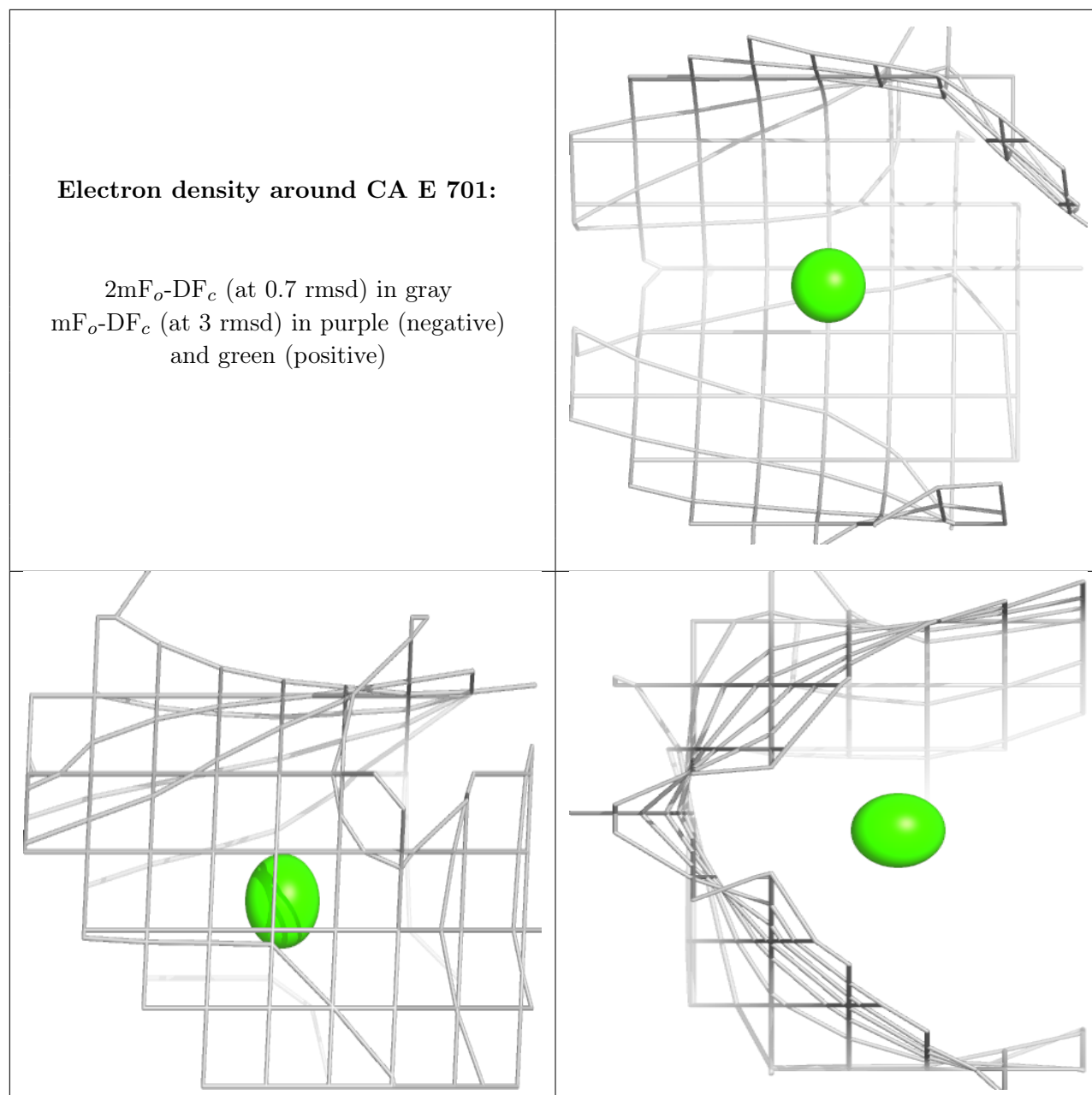
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA G 701:

$2mF_o-DF_c$ (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.