



Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 04:42 PM JST

PDB ID : 9W1H / pdb_00009w1h
EMDB ID : EMD-65540
Title : structure of the type III CRISPR-associated deaminase in complex cA6 and ATP, State 4
Authors : Li, Z.X.; Kong, J.P.; Wu, W.Q.
Deposited on : 2025-07-25
Resolution : 2.94 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

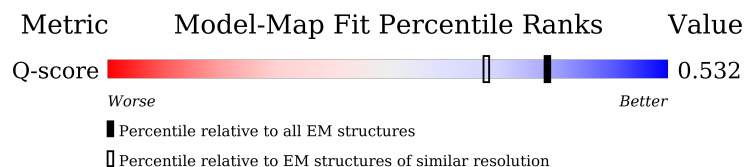
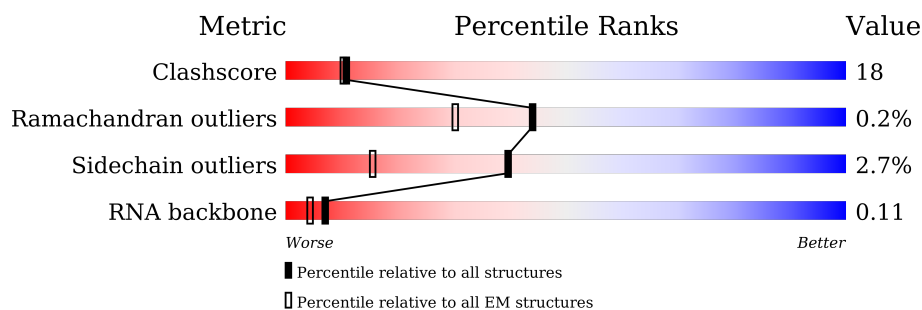
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13068 (2.44 - 3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	631	
1	B	631	
1	C	631	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	631	<div><div><div></div><div></div><div></div></div><div><div>66%</div><div>30%</div><div></div></div></div>
1	E	631	<div><div><div></div><div></div><div></div></div><div><div>38%</div><div>23%</div><div>39%</div></div></div>
1	F	631	<div><div><div></div><div></div><div></div></div><div><div>40%</div><div>22%</div><div>38%</div></div></div>
2	X	6	<div><div><div></div><div></div><div></div></div><div><div>17%</div><div>83%</div></div></div>
2	Y	6	<div><div><div></div><div></div><div></div></div><div><div>33%</div><div>33%</div><div>33%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25533 atoms, of which 72 are hydrogens and 0 are deuteriums.

In the tables below, 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 adenosine deaminase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	593	Total	C	N	O	S	0	0
			4645	2944	848	833	20		
1	D	610	Total	C	N	O	S	0	0
			4772	3020	871	861	20		
1	A	610	Total	C	N	O	S	0	0
			4775	3022	871	861	21		
1	E	388	Total	C	N	O	S	0	0
			3015	1905	553	546	11		
1	F	392	Total	C	N	O	S	0	0
			3035	1918	554	552	11		
1	B	609	Total	C	N	O	S	0	0
			4757	3011	867	858	21		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	626	HIS	-	expression tag	UNP A0A062XY19
C	627	HIS	-	expression tag	UNP A0A062XY19
C	628	HIS	-	expression tag	UNP A0A062XY19
C	629	HIS	-	expression tag	UNP A0A062XY19
C	630	HIS	-	expression tag	UNP A0A062XY19
C	631	HIS	-	expression tag	UNP A0A062XY19
D	626	HIS	-	expression tag	UNP A0A062XY19
D	627	HIS	-	expression tag	UNP A0A062XY19
D	628	HIS	-	expression tag	UNP A0A062XY19
D	629	HIS	-	expression tag	UNP A0A062XY19
D	630	HIS	-	expression tag	UNP A0A062XY19
D	631	HIS	-	expression tag	UNP A0A062XY19
A	626	HIS	-	expression tag	UNP A0A062XY19
A	627	HIS	-	expression tag	UNP A0A062XY19
A	628	HIS	-	expression tag	UNP A0A062XY19
A	629	HIS	-	expression tag	UNP A0A062XY19
A	630	HIS	-	expression tag	UNP A0A062XY19
A	631	HIS	-	expression tag	UNP A0A062XY19

Continued on next page...

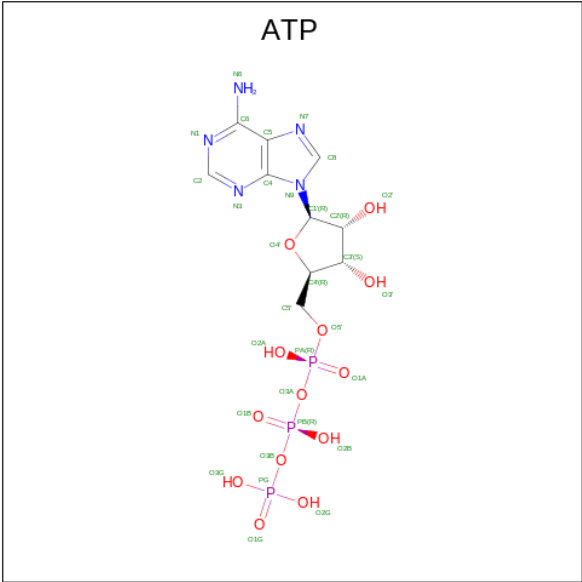
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	626	HIS	-	expression tag	UNP A0A062XY19
E	627	HIS	-	expression tag	UNP A0A062XY19
E	628	HIS	-	expression tag	UNP A0A062XY19
E	629	HIS	-	expression tag	UNP A0A062XY19
E	630	HIS	-	expression tag	UNP A0A062XY19
E	631	HIS	-	expression tag	UNP A0A062XY19
F	626	HIS	-	expression tag	UNP A0A062XY19
F	627	HIS	-	expression tag	UNP A0A062XY19
F	628	HIS	-	expression tag	UNP A0A062XY19
F	629	HIS	-	expression tag	UNP A0A062XY19
F	630	HIS	-	expression tag	UNP A0A062XY19
F	631	HIS	-	expression tag	UNP A0A062XY19
B	626	HIS	-	expression tag	UNP A0A062XY19
B	627	HIS	-	expression tag	UNP A0A062XY19
B	628	HIS	-	expression tag	UNP A0A062XY19
B	629	HIS	-	expression tag	UNP A0A062XY19
B	630	HIS	-	expression tag	UNP A0A062XY19
B	631	HIS	-	expression tag	UNP A0A062XY19

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace
2	X	6	Total	C	N	O	P	
			132	60	30	36	6	0
2	Y	6	Total	C	N	O	P	
			132	60	30	36	6	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	A	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	F	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	

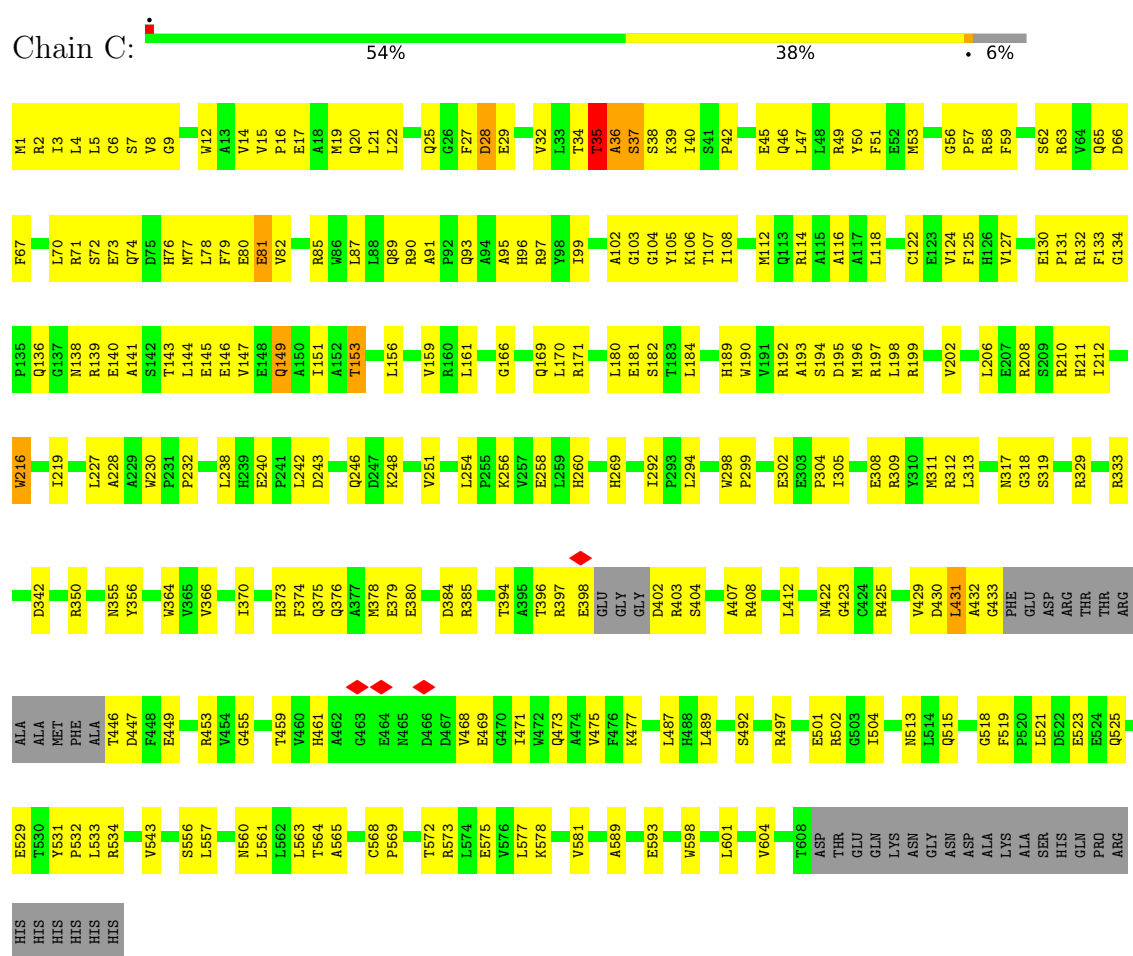
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	

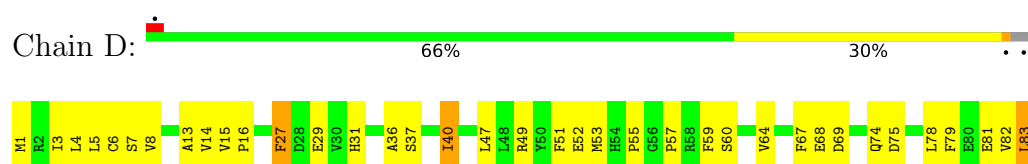
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: adenosine deaminase



- Molecule 1: adenosine deaminase







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.378	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	357.888, 357.888, 357.888	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

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: ZN, ATP, MG

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	0.20	0/4895	0.32	0/6669
1	B	0.20	0/4876	0.31	0/6643
1	C	0.23	0/4761	0.39	2/6486 (0.0%)
1	D	0.21	0/4892	0.31	0/6666
1	E	0.17	0/3089	0.28	0/4215
1	F	0.20	0/3109	0.29	0/4245
2	X	0.19	0/149	0.35	0/230
2	Y	0.18	0/149	0.30	0/230
All	All	0.20	0/25920	0.32	2/35384 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	THR	N-CA-C	10.00	125.98	112.68
1	C	35	THR	CB-CA-C	-6.69	99.07	110.24

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	4775	0	4740	205	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4757	0	4713	191	0
1	C	4645	0	4623	213	0
1	D	4772	0	4733	162	0
1	E	3015	0	3001	110	0
1	F	3035	0	3015	102	0
2	X	132	0	67	10	0
2	Y	132	0	67	7	0
3	A	31	12	12	2	0
3	B	31	12	12	0	0
3	C	31	12	12	1	0
3	D	31	12	12	0	0
3	E	31	12	12	2	0
3	F	31	12	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	25461	72	25031	933	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 18.

All (933) 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:C:469:GLU:HG3	1:A:401:GLY:HA3	1.45	0.97
1:F:431:LEU:HD13	1:F:443:MET:HE3	1.49	0.94
1:E:414:ILE:HG23	1:E:454:VAL:HG21	1.46	0.93
1:A:83:LEU:HD11	1:A:112:MET:HE3	1.52	0.92
1:F:242:LEU:HD23	1:F:565:ALA:HB2	1.51	0.91
1:D:149:GLN:O	1:D:153:THR:HG22	1.72	0.90
1:C:407:ALA:HB1	1:F:450:PRO:HB3	1.54	0.88
1:E:222:LEU:HD13	1:E:223:PRO:HD2	1.53	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:THR:HG22	1:C:63:ARG:HG2	1.58	0.86
1:C:16:PRO:HA	1:C:19:MET:HE3	1.58	0.85
1:D:85:ARG:HB2	1:D:180:LEU:HD13	1.55	0.85
1:C:15:VAL:HG12	1:C:19:MET:HE2	1.60	0.83
1:D:135:PRO:HD2	1:D:139:ARG:HE	1.42	0.82
1:F:277:ARG:HG2	1:F:321:LEU:HD11	1.61	0.81
1:E:407:ALA:HB1	1:B:450:PRO:HB3	1.60	0.81
1:F:219:ILE:HA	1:F:222:LEU:HD23	1.64	0.80
1:C:170:LEU:HD21	1:C:202:VAL:HG22	1.62	0.80
1:B:17:GLU:HB3	1:B:127:VAL:HG21	1.63	0.80
1:E:417:ALA:HB2	1:E:456:LEU:HD21	1.64	0.79
1:E:295:PRO:HG2	1:E:305:ILE:HD11	1.62	0.79
1:D:440:ARG:HG2	1:D:443:MET:HG2	1.65	0.79
1:B:43:GLY:HA2	1:B:46:GLN:HE21	1.48	0.79
1:B:78:LEU:HA	1:B:196:MET:HE1	1.65	0.78
1:D:441:ALA:HB1	1:D:478:LEU:HD22	1.65	0.78
1:E:227:LEU:HD11	1:E:577:LEU:HD23	1.64	0.78
1:D:403:ARG:HD2	1:D:406:ILE:HD12	1.66	0.77
1:F:399:GLU:HB2	1:F:402:ASP:HB2	1.65	0.77
1:B:87:LEU:HD11	1:B:97:ARG:HD3	1.66	0.77
1:B:401:GLY:HA2	1:B:403:ARG:HH22	1.51	0.76
1:C:356:TYR:HB2	1:C:366:VAL:HG11	1.68	0.76
1:A:223:PRO:HG3	1:A:578:LYS:HG3	1.68	0.75
1:A:4:LEU:HD23	1:A:30:VAL:HG13	1.68	0.75
1:D:7:SER:HB3	1:D:112:MET:HE3	1.66	0.75
1:A:459:THR:HG22	1:A:482:ARG:HB2	1.66	0.74
1:A:91:ALA:HB1	1:A:97:ARG:HG2	1.68	0.74
1:A:1:MET:HA	1:A:1:MET:HE2	1.70	0.74
1:B:8:VAL:HB	1:B:34:THR:HG22	1.69	0.74
1:B:544:THR:HG23	1:B:583:ALA:HB2	1.68	0.74
1:C:397:ARG:HB2	1:C:433:GLY:HA3	1.69	0.74
1:D:139:ARG:HH12	1:D:142:SER:HB3	1.54	0.73
1:A:29:GLU:HG3	1:A:58:ARG:HB2	1.70	0.71
1:C:66:ASP:HB2	1:C:78:LEU:HD21	1.71	0.71
1:C:3:ILE:HG21	1:C:91:ALA:HB2	1.72	0.70
1:A:139:ARG:NH1	1:A:140:GLU:O	2.23	0.70
1:D:99:ILE:HD13	1:D:116:ALA:HB2	1.73	0.70
1:F:350:ARG:NH1	1:F:430:ASP:OD2	2.25	0.70
1:B:66:ASP:HB3	1:B:78:LEU:HD21	1.73	0.70
1:E:450:PRO:HB3	1:B:407:ALA:HB1	1.74	0.70
1:F:303:GLU:HG2	1:F:304:PRO:HD2	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HG23	1:A:63:ARG:HG2	1.73	0.70
1:A:304:PRO:HG3	1:A:518:GLY:HA3	1.72	0.70
1:A:441:ALA:HB1	1:A:478:LEU:HD12	1.74	0.70
1:B:251:VAL:HG12	1:B:558:THR:HG23	1.73	0.70
1:C:99:ILE:HD12	1:C:116:ALA:HB2	1.74	0.69
1:C:403:ARG:HH22	1:F:449:GLU:HG2	1.56	0.69
1:C:139:ARG:NH1	1:C:140:GLU:O	2.25	0.69
1:E:260:HIS:CD2	1:E:548:ASP:OD1	2.45	0.69
1:B:327:CYS:O	1:B:329:ARG:N	2.26	0.69
1:C:77:MET:SD	1:C:199:ARG:NH1	2.65	0.69
1:C:22:LEU:HB2	1:C:25:GLN:HE21	1.58	0.69
1:A:16:PRO:HB2	1:A:147:VAL:HG11	1.76	0.68
1:A:15:VAL:HB	1:A:47:LEU:HD11	1.75	0.68
1:E:556:SER:O	1:E:560:ASN:ND2	2.26	0.68
1:E:262:HIS:CD2	1:E:548:ASP:OD1	2.47	0.68
1:C:311:MET:HE2	1:C:311:MET:HA	1.76	0.68
1:D:268:THR:HG23	1:D:314:GLY:HA2	1.76	0.68
1:E:449:GLU:OE2	1:E:453:ARG:NH1	2.27	0.68
1:F:277:ARG:NH2	1:F:287:PRO:O	2.27	0.68
1:F:333:ARG:NH2	1:F:380:GLU:OE1	2.27	0.67
1:A:85:ARG:NH1	1:A:179:PRO:O	2.25	0.67
1:E:240:GLU:HB3	1:E:573:ARG:HH12	1.57	0.67
1:B:165:PRO:O	1:B:171:ARG:NH1	2.27	0.67
1:A:5:LEU:HD11	1:A:91:ALA:HB3	1.76	0.67
1:C:404:SER:OG	1:C:408:ARG:NH1	2.28	0.67
1:A:310:TYR:HH	1:A:553:SER:HG	1.40	0.67
1:E:534:ARG:NH1	1:E:575:GLU:OE2	2.28	0.67
1:C:2:ARG:HG2	1:C:25:GLN:HE22	1.60	0.67
1:D:31:HIS:HD2	1:D:60:SER:HB2	1.60	0.67
1:E:482:ARG:NE	1:E:507:GLU:OE2	2.26	0.67
1:C:228:ALA:HB3	1:D:216:TRP:CH2	2.30	0.67
1:E:243:ASP:OD2	1:E:246:GLN:N	2.23	0.67
1:A:129:CYS:SG	1:A:130:GLU:N	2.67	0.66
1:B:272:LEU:HD13	1:B:334:LEU:HD13	1.76	0.66
1:F:589:ALA:HB1	1:F:593:GLU:HB2	1.76	0.66
1:B:230:TRP:HZ3	1:B:238:LEU:HD13	1.61	0.66
1:D:5:LEU:HD23	1:D:97:ARG:HG2	1.77	0.65
1:C:34:THR:CG2	1:C:63:ARG:HG2	2.25	0.65
1:A:254:LEU:O	1:A:256:LYS:NZ	2.28	0.65
1:E:254:LEU:HD21	1:E:577:LEU:HD11	1.79	0.65
1:C:446:THR:OG1	1:C:447:ASP:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:NE	1:A:507:GLU:OE2	2.27	0.64
1:C:397:ARG:HH11	1:C:431:LEU:HD21	1.63	0.64
1:D:323:LYS:NZ	1:D:357:ALA:O	2.29	0.64
1:E:528:SER:OG	1:E:529:GLU:OE1	2.14	0.64
1:C:21:LEU:HG	1:C:22:LEU:HD23	1.79	0.64
1:A:216:TRP:O	1:A:217:GLU:C	2.41	0.64
1:E:254:LEU:O	1:E:256:LYS:NZ	2.30	0.64
1:B:134:GLY:HA2	1:B:139:ARG:HH11	1.63	0.64
1:B:135:PRO:HD2	1:B:139:ARG:HD3	1.79	0.64
1:F:510:PRO:HD2	1:F:560:ASN:HB3	1.78	0.64
1:D:435:GLU:HB3	1:D:464:GLU:HB3	1.78	0.64
1:E:533:LEU:HD13	1:E:543:VAL:HG11	1.79	0.64
1:C:96:HIS:ND1	1:C:122:CYS:SG	2.70	0.63
1:A:418:GLU:OE1	1:A:418:GLU:N	2.31	0.63
1:D:482:ARG:NE	1:D:507:GLU:OE2	2.26	0.63
1:C:455:GLY:HA3	1:D:497:ARG:HH12	1.64	0.63
1:D:5:LEU:HD21	1:D:91:ALA:HB2	1.79	0.63
1:A:140:GLU:OE2	2:X:6:A:O2'	2.17	0.63
1:B:65:GLN:HB3	1:B:192:ARG:HD3	1.80	0.63
1:C:81:GLU:HB2	1:C:196:MET:HE3	1.80	0.63
1:A:468:VAL:HG13	1:A:495:LEU:HD22	1.81	0.63
1:A:149:GLN:HA	1:A:152:ALA:HB3	1.81	0.62
1:F:227:LEU:HD21	1:F:604:VAL:HG21	1.80	0.62
1:F:449:GLU:OE2	1:F:453:ARG:NH1	2.32	0.62
1:C:85:ARG:HB2	1:C:180:LEU:HD13	1.79	0.62
1:D:15:VAL:HB	1:D:47:LEU:HD11	1.81	0.62
1:D:251:VAL:HG12	1:D:558:THR:HG23	1.82	0.62
1:C:21:LEU:HD23	1:C:27:PHE:HZ	1.65	0.62
1:E:432:ALA:HA	1:E:461:HIS:HB2	1.82	0.62
1:B:547:THR:HG23	1:B:557:LEU:HD13	1.82	0.62
1:C:304:PRO:HG3	1:C:518:GLY:HA3	1.82	0.62
1:A:475:VAL:HG22	1:A:504:ILE:HD13	1.82	0.62
1:F:394:THR:HA	1:F:430:ASP:HB3	1.81	0.61
1:E:329:ARG:O	1:E:333:ARG:HG2	2.00	0.61
1:A:397:ARG:HA	1:A:406:ILE:HD11	1.83	0.61
1:C:408:ARG:NE	1:F:418:GLU:OE1	2.33	0.61
1:C:577:LEU:HD21	1:C:604:VAL:HG11	1.81	0.61
1:B:126:HIS:HB3	1:B:159:VAL:HG13	1.82	0.61
1:D:414:ILE:HG23	1:D:454:VAL:HG21	1.81	0.61
1:C:374:PHE:O	1:C:378:MET:HG3	2.01	0.61
1:A:128:LEU:HD11	1:B:70:LEU:HD23	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:GLU:OE1	1:E:464:GLU:N	2.34	0.60
1:B:227:LEU:HD11	1:B:577:LEU:HD23	1.83	0.60
1:C:133:PHE:CE1	1:C:149:GLN:HG3	2.35	0.60
1:C:556:SER:O	1:C:560:ASN:ND2	2.32	0.60
1:C:589:ALA:HB1	1:C:593:GLU:HB2	1.83	0.60
1:C:513:ASN:ND2	1:C:531:TYR:OH	2.35	0.60
1:C:502:ARG:NH2	1:D:479:SER:O	2.35	0.60
1:B:398:GLU:CB	1:B:439:THR:HB	2.31	0.59
1:C:216:TRP:CZ3	1:D:228:ALA:HB3	2.36	0.59
1:C:561:LEU:O	1:C:564:THR:OG1	2.20	0.59
1:E:435:GLU:HB2	1:E:464:GLU:HB3	1.84	0.59
1:C:407:ALA:CB	1:F:450:PRO:HB3	2.30	0.59
1:A:432:ALA:HA	1:A:461:HIS:HB2	1.85	0.59
1:D:15:VAL:HG21	1:D:47:LEU:HD21	1.84	0.59
1:C:4:LEU:CD1	1:C:6:CYS:HB2	2.33	0.59
1:A:228:ALA:HB3	1:B:216:TRP:CH2	2.36	0.59
1:B:432:ALA:HA	1:B:461:HIS:HB3	1.85	0.59
1:C:196:MET:HE1	1:C:199:ARG:HD3	1.83	0.59
1:B:73:GLU:N	1:B:73:GLU:OE1	2.35	0.59
1:B:85:ARG:HH11	1:B:193:ALA:HB1	1.66	0.59
1:C:581:VAL:HG13	1:C:598:TRP:HH2	1.68	0.59
1:D:81:GLU:OE1	1:D:196:MET:HA	2.03	0.59
1:D:143:THR:N	1:D:146:GLU:OE1	2.35	0.59
1:D:254:LEU:O	1:D:256:LYS:NZ	2.31	0.59
1:D:524:GLU:HB2	1:D:525:GLN:OE1	2.03	0.58
1:F:440:ARG:HH22	1:F:465:ASN:HB3	1.67	0.58
1:A:64:VAL:HG22	1:A:82:VAL:HG11	1.84	0.58
1:A:65:GLN:HB3	1:A:190:TRP:HE3	1.67	0.58
1:B:266:PHE:O	1:B:331:GLN:NE2	2.36	0.58
1:D:133:PHE:HZ	1:D:153:THR:HG21	1.66	0.58
1:A:571:ILE:HG13	1:A:575:GLU:OE1	2.03	0.58
1:D:8:VAL:HG12	1:D:14:VAL:HG23	1.85	0.58
1:A:143:THR:O	1:A:147:VAL:HG23	2.03	0.58
1:E:348:GLU:HG2	1:E:392:LEU:HG	1.85	0.58
1:B:393:LEU:HD12	1:B:413:ALA:HB2	1.84	0.58
1:C:79:PHE:CE2	1:C:108:ILE:HG13	2.38	0.58
1:C:342:ASP:OD2	1:C:556:SER:HB2	2.04	0.58
1:E:248:LYS:HA	1:E:562:LEU:HD11	1.85	0.58
1:E:575:GLU:O	1:E:579:THR:HG23	2.04	0.58
1:E:459:THR:OG1	1:E:482:ARG:HB2	2.04	0.58
1:C:533:LEU:HB3	1:C:568:CYS:SG	2.43	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:556:SER:O	1:F:560:ASN:ND2	2.37	0.58
1:D:397:ARG:HD3	1:D:431:LEU:HD11	1.86	0.58
1:A:34:THR:CG2	1:A:63:ARG:HG2	2.33	0.58
1:A:85:ARG:HB2	1:A:180:LEU:HD13	1.85	0.58
1:B:15:VAL:HB	1:B:16:PRO:HD3	1.86	0.58
1:C:534:ARG:NH1	1:C:569:PRO:O	2.37	0.57
1:D:136:GLN:HE22	1:D:138:ASN:HB3	1.69	0.57
1:A:254:LEU:HD12	1:A:605:PRO:HD2	1.86	0.57
1:B:174:SER:HB2	1:B:176:PRO:HD2	1.85	0.57
1:D:454:VAL:HG13	1:A:408:ARG:NH1	2.19	0.57
1:A:99:ILE:HD12	1:A:116:ALA:HB2	1.87	0.57
1:C:17:GLU:HB3	1:C:127:VAL:HG21	1.85	0.57
1:C:468:VAL:HG21	1:C:492:SER:HB2	1.87	0.57
1:A:29:GLU:CG	1:A:58:ARG:HB2	2.35	0.57
1:E:322:LEU:HD22	1:E:328:LEU:HA	1.86	0.57
1:B:34:THR:OG1	1:B:63:ARG:HG2	2.05	0.57
1:E:531:TYR:HB3	1:E:568:CYS:SG	2.45	0.57
1:A:140:GLU:HB2	2:X:5:A:C6	2.40	0.57
1:C:105:TYR:HB2	1:C:108:ILE:HD13	1.85	0.57
1:C:67:PHE:CD2	1:C:79:PHE:HB2	2.40	0.57
1:C:375:GLN:O	1:C:379:GLU:HG2	2.04	0.57
1:D:374:PHE:O	1:D:378:MET:HG3	2.05	0.57
1:A:237:TRP:O	1:A:573:ARG:NH1	2.37	0.57
1:F:273:LEU:O	1:F:277:ARG:HG3	2.05	0.57
1:D:149:GLN:O	1:D:153:THR:CG2	2.50	0.57
1:D:475:VAL:HG22	1:D:504:ILE:HD13	1.86	0.57
1:A:41:SER:O	1:A:45:GLU:HG2	2.04	0.57
1:F:524:GLU:HB2	1:F:525:GLN:OE1	2.05	0.57
1:B:181:GLU:N	1:B:181:GLU:OE1	2.38	0.56
1:B:447:ASP:OD1	1:B:449:GLU:HB2	2.05	0.56
1:C:89:GLN:HG2	1:C:90:ARG:HD3	1.86	0.56
1:D:101:LEU:HD23	1:D:124:VAL:HG12	1.87	0.56
1:D:223:PRO:HB2	1:D:581:VAL:HG21	1.87	0.56
1:F:284:GLU:OE1	1:F:284:GLU:N	2.35	0.56
1:B:33:LEU:HD12	1:B:86:TRP:CE3	2.41	0.56
1:C:28:ASP:N	1:C:28:ASP:OD1	2.38	0.56
1:A:57:PRO:HG2	1:A:59:PHE:CE1	2.41	0.56
1:F:238:LEU:HD23	1:F:574:LEU:HD13	1.86	0.56
1:B:537:LEU:HD23	1:B:575:GLU:HG2	1.86	0.56
1:E:450:PRO:HB3	1:B:407:ALA:CB	2.36	0.56
1:B:65:GLN:HB3	1:B:192:ARG:CG	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LYS:HD3	1:D:106:LYS:HD2	1.86	0.56
1:D:57:PRO:HG2	1:D:59:PHE:CE1	2.40	0.56
1:E:271:GLU:HG2	1:E:272:LEU:HD22	1.88	0.56
1:F:462:ALA:O	1:F:466:ASP:HB3	2.06	0.56
1:B:489:LEU:HB2	1:B:536:TYR:OH	2.06	0.56
1:C:166:GLY:O	1:C:171:ARG:NH1	2.38	0.56
1:A:34:THR:OG1	1:A:40:ILE:HG21	2.06	0.56
1:B:66:ASP:CB	1:B:78:LEU:HD21	2.36	0.56
1:C:455:GLY:HA3	1:D:497:ARG:NH1	2.20	0.56
1:E:379:GLU:HA	1:E:386:ARG:HH12	1.71	0.56
1:C:105:TYR:CE1	2:Y:6:A:H5''	2.40	0.56
1:F:224:ILE:HG22	1:F:226:ALA:H	1.69	0.56
1:A:33:LEU:HD11	1:A:64:VAL:HG23	1.88	0.56
1:E:254:LEU:HD21	1:E:577:LEU:CD1	2.36	0.56
1:A:43:GLY:HA2	1:A:46:GLN:OE1	2.06	0.55
1:A:258:GLU:HG2	1:A:557:LEU:HD22	1.88	0.55
1:E:361:ARG:NH2	1:E:369:GLU:OE1	2.39	0.55
1:C:2:ARG:HB3	1:C:27:PHE:CD2	2.41	0.55
1:E:547:THR:HG22	1:E:560:ASN:ND2	2.21	0.55
1:C:487:LEU:HD21	1:C:513:ASN:ND2	2.21	0.55
1:C:269:HIS:NE2	1:C:294:LEU:HD21	2.22	0.55
1:E:468:VAL:HG13	1:E:495:LEU:HD22	1.87	0.55
1:C:319:SER:HB3	1:C:355:ASN:HB3	1.89	0.55
1:A:525:GLN:OE1	1:A:525:GLN:N	2.40	0.55
1:B:589:ALA:HB1	1:B:593:GLU:HB2	1.89	0.55
1:A:466:ASP:OD2	1:A:491:ARG:NH2	2.40	0.55
1:B:469:GLU:O	1:B:473:GLN:HG3	2.07	0.55
1:F:533:LEU:HD11	1:F:545:LEU:HD21	1.88	0.55
1:B:374:PHE:O	1:B:378:MET:HG3	2.07	0.55
1:C:350:ARG:NH1	1:C:430:ASP:OD2	2.32	0.55
1:A:234:HIS:CD2	1:A:610:THR:HG21	2.41	0.55
1:F:374:PHE:O	1:F:378:MET:HG3	2.07	0.55
1:C:70:LEU:HD23	1:D:128:LEU:HD21	1.89	0.55
1:C:102:ALA:O	1:D:106:LYS:NZ	2.26	0.55
1:C:159:VAL:HG12	1:C:161:LEU:HD12	1.89	0.55
1:A:471:ILE:CG2	1:A:495:LEU:HD21	2.37	0.55
1:E:296:PRO:HB2	1:E:302:GLU:OE2	2.07	0.55
1:C:230:TRP:HZ3	1:C:238:LEU:HD13	1.71	0.55
1:C:431:LEU:HD13	1:C:433:GLY:H	1.70	0.55
1:A:81:GLU:OE1	1:A:196:MET:HA	2.07	0.55
1:A:91:ALA:CB	1:A:97:ARG:HG2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TYR:OH	1:A:390:ASN:ND2	2.40	0.55
1:C:376:GLN:O	1:C:380:GLU:HG3	2.08	0.54
1:A:15:VAL:O	1:A:19:MET:HG3	2.07	0.54
1:E:310:TYR:OH	1:E:553:SER:OG	2.19	0.54
1:E:576:VAL:O	1:E:579:THR:OG1	2.18	0.54
1:C:138:ASN:OD1	1:C:138:ASN:N	2.40	0.54
1:C:308:GLU:OE2	1:C:312:ARG:NH1	2.40	0.54
1:B:7:SER:HB3	1:B:112:MET:HE3	1.89	0.54
1:B:223:PRO:HD3	1:B:574:LEU:HD11	1.89	0.54
1:A:104:GLY:HA2	2:X:4:A:H1'	1.89	0.54
1:E:356:TYR:HB2	1:E:366:VAL:HG11	1.89	0.54
1:B:333:ARG:O	1:B:337:GLU:HG2	2.07	0.54
1:D:129:CYS:SG	1:D:130:GLU:N	2.78	0.54
1:D:144:LEU:O	1:D:148:GLU:HG2	2.06	0.54
1:A:5:LEU:HD13	1:A:87:LEU:CD1	2.38	0.54
1:D:435:GLU:HB3	1:D:464:GLU:CB	2.38	0.54
1:C:2:ARG:HG2	1:C:25:GLN:NE2	2.21	0.54
1:A:170:LEU:CD2	1:A:202:VAL:HG22	2.38	0.54
1:E:494:ASP:OD1	1:E:494:ASP:N	2.36	0.54
1:C:449:GLU:O	1:C:453:ARG:HG2	2.08	0.53
1:B:126:HIS:HB3	1:B:159:VAL:CG1	2.38	0.53
1:B:280:ALA:HB2	1:B:286:LEU:HD11	1.90	0.53
1:A:132:ARG:NH2	1:A:155:ALA:HB2	2.22	0.53
1:B:1:MET:SD	1:B:1:MET:N	2.75	0.53
1:D:469:GLU:O	1:D:473:GLN:HG3	2.08	0.53
1:C:251:VAL:O	1:C:256:LYS:NZ	2.41	0.53
1:B:5:LEU:HD21	1:B:91:ALA:HB2	1.91	0.53
1:F:489:LEU:HB2	1:F:536:TYR:OH	2.08	0.53
1:A:218:GLY:O	1:A:221:GLU:HG3	2.08	0.53
1:F:576:VAL:O	1:F:579:THR:OG1	2.23	0.53
1:B:85:ARG:NH1	1:B:193:ALA:HB1	2.24	0.53
1:C:62:SER:HA	1:C:189:HIS:O	2.08	0.53
1:C:76:HIS:CE1	1:C:107:THR:HB	2.44	0.53
1:D:268:THR:CG2	1:D:314:GLY:HA2	2.38	0.53
1:A:20:GLN:HG3	1:A:151:ILE:HG22	1.90	0.53
1:F:417:ALA:HB2	1:F:456:LEU:HD21	1.91	0.53
1:B:49:ARG:HA	1:B:52:GLU:OE1	2.08	0.53
1:D:98:TYR:CD2	1:D:123:GLU:HB3	2.44	0.53
1:D:292:ILE:HD11	1:D:315:ASP:HB2	1.90	0.53
1:D:408:ARG:NE	1:A:418:GLU:OE2	2.42	0.53
1:E:475:VAL:HG13	1:E:504:ILE:HD11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:C	1:C:2:ARG:HD2	2.34	0.53
1:C:5:LEU:HG	1:C:87:LEU:HD12	1.90	0.53
1:A:123:GLU:OE1	1:A:124:VAL:N	2.42	0.53
1:F:248:LYS:HD3	1:F:562:LEU:CD1	2.39	0.53
1:B:330:ALA:O	1:B:334:LEU:HG	2.09	0.53
1:B:463:GLY:O	1:B:465:ASN:N	2.42	0.53
1:C:7:SER:O	1:C:103:GLY:HA2	2.09	0.52
1:C:65:GLN:HB3	1:C:190:TRP:HE3	1.73	0.52
1:D:7:SER:HB3	1:D:112:MET:CE	2.37	0.52
1:D:218:GLY:O	1:D:221:GLU:HG3	2.10	0.52
1:C:397:ARG:NH1	1:C:431:LEU:HD21	2.25	0.52
1:C:502:ARG:NH2	1:D:479:SER:HB3	2.24	0.52
1:D:16:PRO:HD3	1:D:47:LEU:HD11	1.90	0.52
1:F:305:ILE:O	1:F:309:ARG:HB2	2.09	0.52
1:B:404:SER:HB3	1:B:408:ARG:NH1	2.23	0.52
1:C:35:THR:O	1:C:36:ALA:CB	2.57	0.52
1:C:184:LEU:HG	1:C:189:HIS:HD2	1.73	0.52
1:A:133:PHE:CE2	1:A:149:GLN:HB2	2.44	0.52
1:C:70:LEU:HB2	1:C:105:TYR:CE2	2.43	0.52
1:C:329:ARG:O	1:C:333:ARG:HG3	2.10	0.52
1:A:5:LEU:HD13	1:A:87:LEU:HD12	1.92	0.52
1:F:251:VAL:HG21	1:F:562:LEU:HD21	1.92	0.52
1:F:575:GLU:O	1:F:579:THR:HG23	2.08	0.52
1:D:8:VAL:HG12	1:D:14:VAL:CG2	2.40	0.52
1:A:218:GLY:O	1:A:219:ILE:C	2.49	0.52
1:A:65:GLN:HB3	1:A:190:TRP:CE3	2.44	0.52
1:F:219:ILE:HD11	1:F:228:ALA:HA	1.92	0.52
1:C:37:SER:O	1:C:38:SER:C	2.52	0.52
1:A:118:LEU:HD22	1:A:206:LEU:HD11	1.90	0.52
1:F:376:GLN:HG2	1:F:380:GLU:OE2	2.10	0.52
1:B:37:SER:HB3	1:B:40:ILE:HD13	1.92	0.52
1:D:143:THR:O	1:D:147:VAL:HG23	2.09	0.52
1:D:375:GLN:O	1:D:379:GLU:HG2	2.09	0.52
1:A:71:ARG:HD3	1:B:157:ARG:CD	2.40	0.52
1:A:218:GLY:C	1:A:220:SER:N	2.62	0.52
1:F:572:THR:OG1	1:F:573:ARG:N	2.43	0.52
1:B:494:ASP:OD1	1:B:494:ASP:N	2.41	0.52
1:D:99:ILE:HD13	1:D:116:ALA:CB	2.39	0.51
1:D:361:ARG:NH2	1:D:369:GLU:OE1	2.43	0.51
1:E:310:TYR:CD2	1:E:516:ILE:HD11	2.45	0.51
2:X:6:A:OP1	1:B:106:LYS:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:LEU:O	1:B:564:THR:OG1	2.27	0.51
1:D:4:LEU:HD13	1:D:27:PHE:CE2	2.45	0.51
1:D:299:PRO:HB3	1:D:553:SER:O	2.10	0.51
1:A:258:GLU:OE1	1:A:261:CYS:HB2	2.10	0.51
1:F:471:ILE:HG22	1:F:495:LEU:HD11	1.91	0.51
1:E:526:GLU:OE1	1:E:526:GLU:N	2.41	0.51
1:C:260:HIS:HA	1:C:350:ARG:HE	1.75	0.51
1:D:237:TRP:HB2	1:D:610:THR:HG23	1.91	0.51
1:D:581:VAL:HG13	1:D:598:TRP:CH2	2.46	0.51
1:A:364:TRP:NE1	1:A:368:GLN:OE1	2.43	0.51
1:B:74:GLN:OE1	1:B:74:GLN:N	2.42	0.51
1:A:81:GLU:CD	1:A:196:MET:HA	2.36	0.51
1:B:17:GLU:N	1:B:17:GLU:OE1	2.43	0.51
1:B:236:ARG:O	1:B:240:GLU:HG2	2.11	0.51
1:C:227:LEU:HD11	1:C:577:LEU:HD23	1.93	0.51
1:D:132:ARG:HH22	1:D:153:THR:HG21	1.75	0.51
1:D:346:TYR:HB2	1:D:597:LEU:HD13	1.92	0.51
1:A:209:SER:HA	1:B:213:LEU:HD21	1.92	0.51
1:A:472:TRP:HB3	1:B:453:ARG:NH1	2.26	0.51
1:E:378:MET:O	1:E:386:ARG:NH1	2.43	0.51
1:E:454:VAL:HA	1:B:408:ARG:NH2	2.26	0.51
1:C:104:GLY:HA2	2:Y:1:A:H1'	1.92	0.51
1:C:256:LYS:HD2	1:C:557:LEU:HD23	1.91	0.51
2:X:2:A:O2'	2:X:3:A:H5'	2.11	0.51
1:B:251:VAL:O	1:B:256:LYS:NZ	2.43	0.51
1:C:38:SER:O	1:C:39:LYS:C	2.54	0.51
1:C:6:CYS:O	1:C:32:VAL:HA	2.11	0.51
1:C:141:ALA:HA	1:C:146:GLU:OE1	2.11	0.51
1:D:432:ALA:HA	1:D:461:HIS:HB2	1.93	0.51
1:A:247:ASP:O	1:A:251:VAL:HG23	2.11	0.51
1:C:398:GLU:HG3	1:C:402:ASP:HB3	1.93	0.50
1:A:118:LEU:CD2	1:A:206:LEU:HD11	2.40	0.50
1:C:21:LEU:HB3	1:C:27:PHE:CZ	2.46	0.50
1:D:130:GLU:HG2	1:D:155:ALA:O	2.11	0.50
1:A:524:GLU:HG2	1:A:525:GLN:OE1	2.10	0.50
1:E:261:CYS:HA	1:E:548:ASP:O	2.12	0.50
1:E:524:GLU:HG3	1:E:525:GLN:OE1	2.11	0.50
1:B:65:GLN:HB3	1:B:192:ARG:CD	2.42	0.50
1:A:2:ARG:HE	1:A:22:LEU:HD13	1.77	0.50
1:B:463:GLY:O	1:B:464:GLU:HG3	2.11	0.50
1:C:78:LEU:O	1:C:82:VAL:HG22	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ALA:HB1	1:A:286:LEU:HD11	1.92	0.50
1:A:388:HIS:NE2	1:A:593:GLU:OE2	2.45	0.50
1:B:312:ARG:HD3	1:B:315:ASP:OD2	2.11	0.50
1:C:195:ASP:CG	1:C:197:ARG:HG3	2.37	0.50
1:C:242:LEU:HD23	1:C:565:ALA:HB2	1.93	0.50
1:A:33:LEU:HD11	1:A:64:VAL:CG2	2.41	0.50
1:C:256:LYS:HB3	1:C:557:LEU:HD23	1.93	0.50
1:F:298:TRP:CG	1:F:299:PRO:HA	2.47	0.50
1:B:268:THR:O	1:B:273:LEU:HD22	2.12	0.50
1:C:147:VAL:O	1:C:151:ILE:HG12	2.12	0.50
1:A:133:PHE:O	1:A:139:ARG:HG3	2.10	0.50
1:A:133:PHE:CZ	1:A:149:GLN:HB2	2.46	0.50
1:A:346:TYR:CE2	1:A:587:ALA:HB1	2.47	0.50
1:B:33:LEU:HD23	1:B:34:THR:N	2.26	0.50
1:D:447:ASP:O	1:D:450:PRO:HD2	2.12	0.50
1:E:376:GLN:O	1:E:380:GLU:HG3	2.12	0.50
1:F:496:LEU:HD11	1:F:541:VAL:HG21	1.93	0.50
2:X:2:A:H5"	1:B:103:GLY:HA2	1.93	0.50
1:B:195:ASP:OD1	1:B:195:ASP:N	2.45	0.50
1:B:237:TRP:O	1:B:573:ARG:NH1	2.45	0.50
1:A:131:PRO:HD3	2:X:6:A:C8	2.47	0.49
1:E:507:GLU:HB3	1:E:546:ASN:ND2	2.25	0.49
1:B:350:ARG:HD3	1:B:430:ASP:OD2	2.12	0.49
1:B:471:ILE:CG2	1:B:495:LEU:HD21	2.41	0.49
1:C:350:ARG:HD3	1:C:430:ASP:OD2	2.11	0.49
1:A:40:ILE:HG22	1:A:44:VAL:HG13	1.93	0.49
1:D:106:LYS:NZ	2:Y:2:A:H5"	2.27	0.49
1:D:310:TYR:HH	1:D:553:SER:HG	1.37	0.49
1:A:29:GLU:OE2	1:A:58:ARG:HD2	2.12	0.49
1:A:118:LEU:HD13	1:A:202:VAL:HG11	1.93	0.49
1:A:436:ASP:OD1	1:A:439:THR:OG1	2.18	0.49
1:A:469:GLU:OE2	1:B:453:ARG:NH2	2.45	0.49
1:E:237:TRP:CE3	1:E:607:PRO:HG3	2.47	0.49
1:D:123:GLU:OE2	1:D:160:ARG:NE	2.32	0.49
1:A:53:MET:HG3	1:A:54:HIS:HD2	1.78	0.49
1:A:80:GLU:OE2	1:A:114:ARG:NH1	2.45	0.49
1:C:82:VAL:HG12	1:C:193:ALA:HB2	1.94	0.49
1:D:67:PHE:CD1	1:D:79:PHE:HB2	2.48	0.49
1:E:318:GLY:HA3	3:E:701:ATP:O2B	2.12	0.49
1:E:416:ALA:HB1	1:E:426:VAL:HG21	1.93	0.49
1:E:466:ASP:OD1	1:E:466:ASP:N	2.35	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:ALA:HB1	1:E:593:GLU:HB2	1.93	0.49
1:F:243:ASP:OD1	1:F:246:GLN:N	2.23	0.49
1:B:143:THR:O	1:B:147:VAL:HG12	2.12	0.49
1:D:531:TYR:HB3	1:D:568:CYS:SG	2.53	0.49
1:A:141:ALA:O	2:X:5:A:N6	2.37	0.49
1:A:581:VAL:HG13	1:A:598:TRP:HH2	1.77	0.49
1:B:444:PHE:CE1	1:B:478:LEU:HG	2.47	0.49
1:C:20:GLN:N	1:C:20:GLN:OE1	2.45	0.49
1:A:581:VAL:HG13	1:A:598:TRP:CH2	2.48	0.49
1:F:471:ILE:CG2	1:F:495:LEU:HD21	2.43	0.49
1:B:223:PRO:HD2	1:B:227:LEU:HD12	1.95	0.49
1:B:317:ASN:ND2	1:B:331:GLN:OE1	2.42	0.49
1:B:497:ARG:NH1	1:B:501:GLU:OE2	2.46	0.49
1:C:531:TYR:HB3	1:C:568:CYS:SG	2.53	0.49
1:D:124:VAL:O	1:D:161:LEU:HB2	2.13	0.49
1:D:436:ASP:OD1	1:D:439:THR:OG1	2.17	0.49
1:D:15:VAL:HB	1:D:16:PRO:HD3	1.94	0.49
1:B:14:VAL:CG1	1:B:102:ALA:HB3	2.43	0.49
1:B:217:GLU:CD	1:B:217:GLU:H	2.21	0.49
1:D:396:THR:HG23	1:D:433:GLY:CA	2.43	0.48
1:A:40:ILE:HD12	1:A:40:ILE:H	1.78	0.48
1:A:149:GLN:O	1:A:153:THR:HG23	2.13	0.48
1:A:449:GLU:HB3	1:A:450:PRO:HD3	1.94	0.48
1:E:303:GLU:OE1	1:E:304:PRO:HD2	2.12	0.48
1:B:28:ASP:O	1:B:29:GLU:HG3	2.13	0.48
1:B:93:GLN:HB3	1:B:96:HIS:CE1	2.48	0.48
1:B:246:GLN:N	1:B:246:GLN:OE1	2.46	0.48
1:B:587:ALA:O	1:B:594:ARG:NH2	2.46	0.48
1:C:144:LEU:HD12	1:C:144:LEU:H	1.77	0.48
1:D:305:ILE:O	1:D:309:ARG:HB2	2.13	0.48
1:D:581:VAL:HG13	1:D:598:TRP:HH2	1.78	0.48
1:A:466:ASP:HA	1:A:488:HIS:HD2	1.78	0.48
1:E:431:LEU:HB3	1:E:443:MET:SD	2.52	0.48
1:F:231:PRO:HD2	1:F:234:HIS:ND1	2.28	0.48
1:B:254:LEU:O	1:B:256:LYS:NZ	2.43	0.48
1:D:307:LEU:HD23	1:D:464:GLU:HG2	1.95	0.48
1:A:81:GLU:OE2	1:A:196:MET:HA	2.13	0.48
1:A:524:GLU:N	1:A:524:GLU:OE1	2.47	0.48
1:B:5:LEU:HD12	1:B:86:TRP:CH2	2.48	0.48
1:B:34:THR:O	1:B:63:ARG:HA	2.13	0.48
1:B:475:VAL:HG13	1:B:504:ILE:HD11	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:VAL:HG22	1:B:504:ILE:HD13	1.95	0.48
1:E:350:ARG:HB3	1:E:394:THR:OG1	2.13	0.48
1:F:534:ARG:NH1	1:F:570:GLY:O	2.46	0.48
1:B:436:ASP:OD2	1:B:439:THR:HG22	2.13	0.48
1:C:85:ARG:CB	1:C:180:LEU:HD13	2.43	0.48
1:D:183:THR:HG22	1:D:184:LEU:H	1.77	0.48
1:A:440:ARG:HH12	1:A:467:ASP:HB2	1.79	0.48
1:B:60:SER:OG	1:B:90:ARG:NH2	2.46	0.48
1:C:96:HIS:HA	1:C:122:CYS:SG	2.54	0.48
1:A:242:LEU:HD12	1:A:247:ASP:OD2	2.13	0.48
1:A:489:LEU:HB2	1:A:536:TYR:OH	2.13	0.48
1:A:521:LEU:HD12	1:A:567:LEU:HD23	1.96	0.48
1:F:251:VAL:HG12	1:F:558:THR:HG23	1.96	0.48
1:B:65:GLN:HG3	1:B:190:TRP:CE3	2.49	0.48
1:C:143:THR:O	1:C:147:VAL:HG23	2.13	0.48
1:D:31:HIS:HB3	1:D:86:TRP:CZ2	2.49	0.48
1:D:395:ALA:HB1	1:D:406:ILE:HG23	1.96	0.48
1:F:471:ILE:O	1:F:475:VAL:HG13	2.14	0.48
1:B:348:GLU:HA	1:B:390:ASN:O	2.13	0.48
1:B:376:GLN:O	1:B:380:GLU:HG3	2.13	0.48
1:D:520:PRO:O	1:D:521:LEU:HD23	2.13	0.48
1:E:318:GLY:O	1:E:322:LEU:HB2	2.14	0.48
1:E:453:ARG:NH2	1:B:402:ASP:O	2.35	0.48
1:B:482:ARG:NE	1:B:507:GLU:OE2	2.33	0.48
1:C:181:GLU:OE2	1:C:194:SER:HB3	2.14	0.48
1:E:243:ASP:O	1:E:247:ASP:HB2	2.14	0.48
1:B:433:GLY:O	1:B:439:THR:HG23	2.14	0.48
1:C:74:GLN:N	1:C:74:GLN:OE1	2.47	0.48
1:A:330:ALA:O	1:A:334:LEU:HG	2.14	0.48
1:E:242:LEU:HD23	1:E:565:ALA:HB2	1.96	0.48
1:F:414:ILE:HG23	1:F:454:VAL:HG11	1.96	0.48
1:B:533:LEU:HD11	1:B:545:LEU:HD21	1.96	0.48
1:C:146:GLU:HA	1:C:149:GLN:OE1	2.14	0.47
1:C:182:SER:HA	1:C:190:TRP:O	2.14	0.47
1:D:74:GLN:OE1	1:D:74:GLN:N	2.47	0.47
1:D:91:ALA:HB1	1:D:97:ARG:HG3	1.95	0.47
1:A:110:ALA:HB1	1:B:113:GLN:OE1	2.14	0.47
1:A:130:GLU:HG2	1:A:132:ARG:H	1.78	0.47
1:E:399:GLU:HB2	1:E:439:THR:HG23	1.96	0.47
1:A:181:GLU:OE1	1:A:192:ARG:HD2	2.15	0.47
1:E:350:ARG:HD3	1:E:430:ASP:OD2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:HD22	1:B:202:VAL:HG22	1.96	0.47
1:C:21:LEU:HD22	1:C:125:PHE:CE1	2.49	0.47
1:C:329:ARG:NH1	1:C:333:ARG:HD2	2.29	0.47
1:D:364:TRP:NE1	1:D:368:GLN:OE1	2.47	0.47
1:D:466:ASP:HB3	1:D:491:ARG:HH12	1.79	0.47
1:A:50:TYR:HA	1:A:53:MET:HE2	1.96	0.47
1:A:280:ALA:CB	1:A:286:LEU:HD11	2.45	0.47
1:E:290:ARG:HH21	1:E:315:ASP:HB3	1.78	0.47
1:E:550:LEU:HD23	1:E:555:ALA:O	2.14	0.47
1:F:350:ARG:HD3	1:F:430:ASP:OD2	2.14	0.47
1:D:31:HIS:CD2	1:D:60:SER:HB2	2.44	0.47
1:D:57:PRO:HG2	1:D:59:PHE:CZ	2.49	0.47
1:E:340:LEU:HD21	1:E:385:ARG:O	2.15	0.47
1:B:450:PRO:O	1:B:454:VAL:HG13	2.14	0.47
1:B:526:GLU:HG3	1:B:530:THR:HG21	1.97	0.47
1:C:243:ASP:OD2	1:C:246:GLN:N	2.26	0.47
1:A:15:VAL:CB	1:A:47:LEU:HD11	2.44	0.47
1:A:143:THR:OG1	1:A:146:GLU:HB2	2.14	0.47
1:A:494:ASP:OD1	1:A:497:ARG:NH2	2.48	0.47
1:E:307:LEU:O	1:E:311:MET:HG3	2.15	0.47
1:B:404:SER:HB3	1:B:408:ARG:HH12	1.78	0.47
1:A:85:ARG:NH2	1:A:195:ASP:O	2.48	0.47
1:A:284:GLU:OE1	1:A:284:GLU:N	2.47	0.47
1:A:498:VAL:O	1:A:502:ARG:HG3	2.14	0.47
1:B:242:LEU:HD12	1:B:247:ASP:OD2	2.14	0.47
1:C:2:ARG:HB2	1:C:27:PHE:HA	1.96	0.47
1:C:396:THR:HA	1:C:432:ALA:HB3	1.97	0.47
1:C:423:GLY:O	1:C:425:ARG:HG3	2.15	0.47
1:D:170:LEU:HD21	1:D:205:VAL:HG11	1.95	0.47
1:A:17:GLU:HB3	1:A:156:LEU:HD13	1.95	0.47
1:A:70:LEU:O	1:A:70:LEU:HD23	2.14	0.47
1:A:431:LEU:HD13	1:A:448:PHE:CZ	2.50	0.47
1:E:434:PHE:O	1:E:440:ARG:HD3	2.14	0.47
1:C:228:ALA:HB3	1:D:216:TRP:CZ3	2.49	0.47
1:D:51:PHE:HB3	1:D:59:PHE:CD2	2.49	0.47
1:D:397:ARG:HG2	1:D:444:PHE:CZ	2.50	0.47
1:A:310:TYR:CD2	1:A:516:ILE:HD11	2.49	0.47
1:F:432:ALA:HA	1:F:461:HIS:HB2	1.97	0.47
1:C:134:GLY:HA2	1:C:139:ARG:CZ	2.44	0.47
1:F:590:ASN:OD1	1:F:593:GLU:HG3	2.15	0.47
1:B:310:TYR:CD2	1:B:516:ILE:HD11	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ASP:OD1	1:C:385:ARG:HG3	2.14	0.47
1:E:384:ASP:OD1	1:E:385:ARG:HG3	2.15	0.47
1:E:574:LEU:HD23	1:E:578:LYS:HG3	1.97	0.47
1:F:310:TYR:OH	1:F:553:SER:HB2	2.15	0.47
1:D:507:GLU:HB3	1:D:546:ASN:ND2	2.30	0.46
1:A:374:PHE:O	1:A:378:MET:HG3	2.15	0.46
1:A:555:ALA:HB1	1:A:559:ASP:HB2	1.96	0.46
1:B:9:GLY:O	1:B:40:ILE:HG13	2.15	0.46
1:B:317:ASN:OD1	1:B:318:GLY:N	2.47	0.46
1:A:459:THR:CG2	1:A:482:ARG:HB2	2.41	0.46
1:B:273:LEU:O	1:B:277:ARG:HG3	2.14	0.46
1:C:497:ARG:O	1:C:501:GLU:HG3	2.15	0.46
1:A:13:ALA:C	1:A:16:PRO:HD2	2.40	0.46
1:A:70:LEU:HD11	1:A:107:THR:OG1	2.16	0.46
1:A:216:TRP:HH2	1:B:219:ILE:HD11	1.81	0.46
1:A:263:LEU:O	1:A:331:GLN:NE2	2.47	0.46
1:E:233:SER:O	1:E:236:ARG:HG2	2.15	0.46
1:A:146:GLU:HA	1:A:149:GLN:OE1	2.16	0.46
1:A:237:TRP:CH2	1:A:573:ARG:HD3	2.51	0.46
1:A:318:GLY:HA3	3:A:701:ATP:O2B	2.15	0.46
1:E:263:LEU:O	1:E:331:GLN:NE2	2.49	0.46
1:F:435:GLU:HB3	1:F:464:GLU:HB3	1.98	0.46
1:C:17:GLU:OE2	2:Y:2:A:N6	2.42	0.46
1:D:81:GLU:CD	1:D:196:MET:HA	2.40	0.46
1:D:101:LEU:HD21	1:D:161:LEU:HD22	1.98	0.46
1:A:441:ALA:HB1	1:A:478:LEU:CD1	2.45	0.46
1:E:227:LEU:HD21	1:E:604:VAL:HG11	1.98	0.46
1:E:574:LEU:O	1:E:578:LYS:HG3	2.15	0.46
1:C:15:VAL:HB	1:C:16:PRO:HD3	1.97	0.46
1:C:22:LEU:HD12	1:C:25:GLN:NE2	2.31	0.46
1:C:130:GLU:HG2	1:C:132:ARG:H	1.81	0.46
1:F:230:TRP:CE3	1:F:234:HIS:HB3	2.51	0.46
1:B:98:TYR:CD2	1:B:123:GLU:HB3	2.50	0.46
1:C:2:ARG:HG2	1:C:22:LEU:HD12	1.97	0.46
1:C:258:GLU:OE1	1:C:557:LEU:HD22	2.16	0.46
1:A:53:MET:HG3	1:A:54:HIS:CD2	2.50	0.46
1:B:294:LEU:HD23	1:B:313:LEU:CD2	2.46	0.46
1:B:574:LEU:O	1:B:578:LYS:HG3	2.16	0.46
1:C:72:SER:OG	1:C:73:GLU:N	2.49	0.46
1:C:149:GLN:O	1:C:153:THR:HG23	2.16	0.46
1:A:51:PHE:HE2	1:A:61:ILE:HD11	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:HIS:HB3	1:F:476:PHE:CZ	2.51	0.46
1:B:346:TYR:CE2	1:B:348:GLU:HG3	2.50	0.46
1:B:347:ALA:HB3	1:B:389:VAL:HG22	1.97	0.46
1:D:13:ALA:C	1:D:16:PRO:HD2	2.41	0.46
1:D:376:GLN:O	1:D:380:GLU:HG3	2.16	0.46
1:D:466:ASP:O	1:D:491:ARG:NH2	2.48	0.46
1:D:475:VAL:HG13	1:D:504:ILE:HD11	1.98	0.46
1:A:550:LEU:HD21	1:A:556:SER:HA	1.98	0.46
1:E:379:GLU:HA	1:E:386:ARG:NH1	2.30	0.46
1:B:44:VAL:HG13	1:B:61:ILE:HG21	1.97	0.46
1:B:305:ILE:HD11	1:B:310:TYR:HA	1.98	0.46
1:C:67:PHE:HZ	1:C:70:LEU:HD13	1.81	0.45
1:C:118:LEU:HD21	1:C:206:LEU:HD11	1.97	0.45
1:C:578:LYS:HB2	1:C:578:LYS:HE3	1.68	0.45
1:E:533:LEU:CD1	1:E:543:VAL:HG11	2.46	0.45
1:F:499:VAL:HG12	1:F:541:VAL:HG13	1.97	0.45
1:C:2:ARG:CB	1:C:27:PHE:HA	2.46	0.45
1:C:305:ILE:O	1:C:309:ARG:HB2	2.16	0.45
1:A:317:ASN:OD1	1:A:318:GLY:N	2.49	0.45
1:E:295:PRO:HG2	1:E:305:ILE:CD1	2.40	0.45
1:F:431:LEU:HB2	1:F:460:VAL:HG22	1.98	0.45
1:C:192:ARG:HB3	1:C:192:ARG:NH1	2.31	0.45
1:C:408:ARG:HG2	1:F:418:GLU:OE2	2.16	0.45
1:A:8:VAL:CG1	1:A:15:VAL:HG23	2.46	0.45
1:A:67:PHE:CE2	1:A:75:ASP:HB3	2.51	0.45
1:A:414:ILE:HG23	1:A:454:VAL:HG11	1.97	0.45
1:E:312:ARG:NH1	1:E:315:ASP:OD1	2.50	0.45
1:B:170:LEU:CD2	1:B:202:VAL:HG22	2.46	0.45
1:C:184:LEU:HG	1:C:189:HIS:CD2	2.50	0.45
1:C:366:VAL:O	1:C:370:ILE:HG13	2.16	0.45
2:X:2:A:N1	1:B:17:GLU:HG2	2.31	0.45
1:B:43:GLY:HA2	1:B:46:GLN:NE2	2.26	0.45
1:D:53:MET:O	1:D:55:PRO:HD3	2.17	0.45
1:D:112:MET:HE2	1:D:112:MET:HB2	1.85	0.45
1:D:147:VAL:O	1:D:151:ILE:HG12	2.17	0.45
1:A:4:LEU:HD22	1:A:19:MET:HG2	1.99	0.45
1:E:449:GLU:O	1:E:453:ARG:HG2	2.17	0.45
1:B:13:ALA:HB1	1:B:17:GLU:OE2	2.17	0.45
1:D:440:ARG:HG2	1:D:443:MET:CG	2.41	0.45
1:D:520:PRO:HG2	1:D:529:GLU:O	2.17	0.45
1:A:313:LEU:O	1:A:313:LEU:HD23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LEU:CD1	1:E:605:PRO:HD2	2.47	0.45
1:F:450:PRO:O	1:F:454:VAL:HG22	2.16	0.45
1:B:15:VAL:HB	1:B:47:LEU:HD11	1.98	0.45
1:B:64:VAL:HG22	1:B:82:VAL:HG11	1.97	0.45
1:C:523:GLU:HG2	1:C:525:GLN:OE1	2.17	0.45
1:D:136:GLN:NE2	1:D:138:ASN:HB3	2.29	0.45
1:A:21:LEU:HD13	1:A:125:PHE:CD2	2.51	0.45
1:C:80:GLU:OE1	1:C:114:ARG:NH2	2.48	0.45
1:C:219:ILE:HD13	1:D:219:ILE:HD13	1.98	0.45
1:D:174:SER:HB2	1:D:176:PRO:HD2	1.99	0.45
1:D:317:ASN:OD1	1:D:318:GLY:N	2.50	0.45
1:A:124:VAL:O	1:A:161:LEU:N	2.46	0.45
1:A:149:GLN:O	1:A:153:THR:N	2.43	0.45
1:A:318:GLY:O	1:A:322:LEU:HB2	2.15	0.45
1:E:394:THR:HA	1:E:430:ASP:HB3	1.99	0.45
1:F:264:GLY:HA3	3:F:701:ATP:O2B	2.17	0.45
1:F:342:ASP:OD2	1:F:556:SER:HB2	2.17	0.45
1:B:537:LEU:CD2	1:B:575:GLU:HG2	2.47	0.45
1:C:394:THR:HG21	3:C:701:ATP:H4'	1.99	0.45
1:C:404:SER:HG	1:C:408:ARG:HH11	1.64	0.45
1:E:286:LEU:HD22	1:E:321:LEU:CD1	2.47	0.45
1:E:533:LEU:HB3	1:E:568:CYS:SG	2.56	0.45
1:F:531:TYR:CD1	1:F:532:PRO:HD2	2.51	0.45
1:C:468:VAL:HG21	1:C:492:SER:CB	2.47	0.44
1:D:428:GLY:HA2	1:D:456:LEU:HD22	1.99	0.44
1:A:358:SER:OG	1:A:361:ARG:HG3	2.17	0.44
1:A:531:TYR:CD1	1:A:532:PRO:HD2	2.53	0.44
1:F:219:ILE:HD12	1:F:222:LEU:HG	1.99	0.44
1:F:435:GLU:OE2	1:F:461:HIS:HB3	2.15	0.44
1:B:178:PHE:HE1	1:B:197:ARG:HG2	1.81	0.44
1:C:292:ILE:HG21	1:C:313:LEU:O	2.17	0.44
1:A:53:MET:C	1:A:55:PRO:HD3	2.42	0.44
1:E:317:ASN:OD1	1:E:318:GLY:N	2.51	0.44
1:B:276:VAL:HG12	1:B:321:LEU:HD21	1.99	0.44
1:B:468:VAL:HG12	1:B:472:TRP:CD1	2.52	0.44
1:C:531:TYR:CD1	1:C:532:PRO:HD2	2.53	0.44
1:D:407:ALA:HB1	1:A:450:PRO:HB3	2.00	0.44
1:D:509:CYS:SG	1:D:548:ASP:HB2	2.58	0.44
1:E:521:LEU:HD12	1:E:521:LEU:HA	1.81	0.44
1:E:550:LEU:CD2	1:E:556:SER:HA	2.47	0.44
1:F:251:VAL:CG1	1:F:558:THR:HG23	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:CE2	1:B:108:ILE:HD12	2.53	0.44
1:B:84:TRP:HB3	1:B:198:LEU:HD23	2.00	0.44
1:B:364:TRP:NE1	1:B:368:GLN:OE1	2.49	0.44
1:D:397:ARG:O	1:D:434:PHE:N	2.41	0.44
1:E:366:VAL:O	1:E:370:ILE:HG13	2.18	0.44
1:F:425:ARG:NH1	1:F:593:GLU:OE2	2.50	0.44
1:B:31:HIS:CG	1:B:90:ARG:HG3	2.53	0.44
1:C:254:LEU:O	1:C:256:LYS:NZ	2.40	0.44
1:C:256:LYS:HB3	1:C:557:LEU:CD2	2.48	0.44
1:C:397:ARG:CD	1:C:433:GLY:HA3	2.47	0.44
1:A:218:GLY:O	1:A:220:SER:N	2.51	0.44
1:B:62:SER:HA	1:B:189:HIS:O	2.16	0.44
1:C:105:TYR:CD1	2:Y:6:A:H5''	2.53	0.44
1:D:139:ARG:HH12	1:D:142:SER:CB	2.26	0.44
1:A:5:LEU:HD11	1:A:91:ALA:CB	2.44	0.44
1:A:148:GLU:CD	1:A:151:ILE:HD11	2.42	0.44
1:A:184:LEU:HG	1:A:189:HIS:CD2	2.52	0.44
1:A:223:PRO:HB2	1:A:224:ILE:HD12	1.99	0.44
1:F:255:PRO:HB2	1:F:601:LEU:HD12	2.00	0.44
1:B:134:GLY:CA	1:B:139:ARG:HH11	2.30	0.44
1:B:471:ILE:HG21	1:B:495:LEU:HD21	1.99	0.44
1:C:2:ARG:O	1:C:27:PHE:HB3	2.18	0.44
1:C:12:TRP:NE1	1:C:46:GLN:OE1	2.51	0.44
1:A:65:GLN:HG2	1:A:191:VAL:O	2.17	0.44
1:A:124:VAL:O	1:A:161:LEU:HB2	2.17	0.44
1:A:432:ALA:HB2	1:A:461:HIS:ND1	2.33	0.44
1:A:455:GLY:HA3	1:B:497:ARG:NH2	2.32	0.44
1:F:281:ALA:HB3	1:F:324:ASP:OD1	2.18	0.44
1:B:66:ASP:OD2	1:B:192:ARG:HD2	2.18	0.44
1:B:434:PHE:CD1	1:B:440:ARG:HG3	2.53	0.44
1:C:9:GLY:C	1:C:40:ILE:HD12	2.42	0.44
1:D:83:LEU:HD11	1:D:112:MET:SD	2.57	0.44
1:D:237:TRP:CZ3	1:D:607:PRO:HB3	2.53	0.44
1:D:396:THR:HG23	1:D:433:GLY:HA2	2.00	0.44
1:D:517:LYS:HE2	1:D:517:LYS:HB2	1.83	0.44
1:C:130:GLU:HG3	1:C:131:PRO:HD2	2.00	0.43
1:C:329:ARG:HB2	1:C:373:HIS:CE1	2.53	0.43
1:A:17:GLU:HG2	1:A:156:LEU:HD11	1.99	0.43
1:E:294:LEU:HD23	1:E:313:LEU:HD22	2.00	0.43
1:F:356:TYR:HB2	1:F:366:VAL:HG11	2.00	0.43
1:B:575:GLU:O	1:B:579:THR:HG23	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLU:HG2	1:C:156:LEU:HD21	2.00	0.43
1:C:28:ASP:C	1:C:57:PRO:HB3	2.43	0.43
1:C:49:ARG:O	1:C:53:MET:HG3	2.18	0.43
1:C:57:PRO:HB2	1:C:59:PHE:CE1	2.53	0.43
1:A:16:PRO:CB	1:A:147:VAL:HG11	2.47	0.43
1:B:90:ARG:HD2	1:B:90:ARG:HA	1.76	0.43
1:B:319:SER:HB3	1:B:355:ASN:HB3	2.00	0.43
1:B:509:CYS:SG	1:B:548:ASP:HB2	2.58	0.43
1:C:130:GLU:OE2	1:C:132:ARG:HB2	2.18	0.43
1:F:251:VAL:HG21	1:F:562:LEU:CD2	2.48	0.43
1:F:269:HIS:NE2	1:F:294:LEU:HD11	2.33	0.43
1:B:520:PRO:O	1:B:521:LEU:HD23	2.18	0.43
1:C:131:PRO:HB2	1:C:138:ASN:O	2.18	0.43
1:C:521:LEU:HD21	1:C:563:LEU:HD11	2.00	0.43
1:A:223:PRO:CG	1:A:578:LYS:HG3	2.44	0.43
1:A:455:GLY:HA3	1:B:497:ARG:HH22	1.84	0.43
1:F:275:LYS:HE2	1:F:275:LYS:HB2	1.87	0.43
1:F:529:GLU:OE1	1:F:529:GLU:N	2.52	0.43
1:B:292:ILE:HD11	1:B:315:ASP:HB2	2.01	0.43
1:B:396:THR:OG1	1:B:397:ARG:N	2.52	0.43
1:C:56:GLY:HA3	1:C:57:PRO:HD3	1.81	0.43
1:B:606:VAL:HA	1:B:607:PRO:HD3	1.89	0.43
1:C:93:GLN:HB2	1:C:97:ARG:NH2	2.34	0.43
1:C:487:LEU:HD13	1:C:519:PHE:HZ	1.83	0.43
1:D:67:PHE:O	1:D:69:ASP:N	2.52	0.43
1:A:70:LEU:HD21	1:B:159:VAL:HG11	1.99	0.43
1:E:254:LEU:HD12	1:E:605:PRO:HD2	2.01	0.43
1:F:521:LEU:HD11	1:F:563:LEU:HD11	2.00	0.43
1:B:489:LEU:HB2	1:B:536:TYR:CZ	2.53	0.43
1:A:19:MET:SD	1:A:30:VAL:HG21	2.58	0.43
1:A:70:LEU:HD22	1:B:128:LEU:HD11	2.00	0.43
1:A:371:ARG:HG2	1:A:424:CYS:SG	2.58	0.43
1:A:460:VAL:O	1:A:484:GLY:N	2.44	0.43
1:F:371:ARG:HD2	1:F:420:TRP:CE2	2.54	0.43
1:A:256:LYS:HB3	1:A:557:LEU:HD23	2.00	0.43
1:C:14:VAL:CG1	1:C:102:ALA:HB3	2.48	0.43
1:C:79:PHE:CZ	1:C:108:ILE:HG13	2.53	0.43
1:C:114:ARG:HD3	1:D:113:GLN:HE21	1.84	0.43
1:A:69:ASP:OD1	1:A:105:TYR:OH	2.30	0.43
1:A:126:HIS:CE1	1:B:106:LYS:HB2	2.54	0.43
1:B:72:SER:OG	1:B:73:GLU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:LYS:HE2	1:B:477:LYS:HB2	1.84	0.43
1:C:42:PRO:HA	1:C:45:GLU:OE1	2.19	0.43
1:D:132:ARG:NH2	1:D:153:THR:HG21	2.34	0.43
1:B:13:ALA:O	1:B:16:PRO:HD2	2.18	0.43
1:A:305:ILE:O	1:A:309:ARG:HB2	2.19	0.42
1:B:219:ILE:HD13	1:B:219:ILE:HA	1.90	0.42
1:C:21:LEU:HD23	1:C:27:PHE:CZ	2.50	0.42
1:C:317:ASN:OD1	1:C:318:GLY:N	2.52	0.42
1:C:429:VAL:O	1:C:459:THR:HG22	2.19	0.42
1:C:572:THR:OG1	1:C:575:GLU:HG3	2.18	0.42
1:A:20:GLN:HG3	1:A:151:ILE:CG2	2.49	0.42
1:E:395:ALA:O	1:E:432:ALA:HB3	2.19	0.42
1:F:347:ALA:HB3	1:F:389:VAL:HG22	2.01	0.42
2:X:2:A:H5"	1:B:102:ALA:O	2.18	0.42
1:B:346:TYR:CE2	1:B:587:ALA:HB1	2.53	0.42
1:B:384:ASP:OD1	1:B:385:ARG:HG3	2.19	0.42
1:C:146:GLU:HA	1:C:149:GLN:CD	2.43	0.42
1:C:240:GLU:HB2	1:C:573:ARG:HH12	1.84	0.42
1:D:8:VAL:CG1	1:D:15:VAL:HG23	2.49	0.42
1:D:136:GLN:NE2	1:D:138:ASN:O	2.52	0.42
1:D:148:GLU:HA	1:D:151:ILE:HG12	2.02	0.42
1:D:195:ASP:OD2	1:D:197:ARG:HB2	2.19	0.42
1:E:348:GLU:HA	1:E:390:ASN:O	2.19	0.42
1:E:468:VAL:HG12	1:E:472:TRP:CD1	2.54	0.42
1:E:497:ARG:O	1:E:501:GLU:HG2	2.20	0.42
1:C:124:VAL:O	1:C:161:LEU:HB2	2.19	0.42
1:C:248:LYS:HE3	1:C:248:LYS:HB3	1.89	0.42
1:A:132:ARG:NH2	1:A:153:THR:OG1	2.53	0.42
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.83	0.42
1:F:279:GLU:HB2	1:F:330:ALA:HB2	2.01	0.42
1:F:282:ASN:HB2	1:F:285:SER:OG	2.20	0.42
1:F:294:LEU:HD23	1:F:298:TRP:CD1	2.55	0.42
1:F:364:TRP:HZ3	1:F:416:ALA:HB2	1.85	0.42
1:C:65:GLN:HB3	1:C:190:TRP:CE3	2.53	0.42
1:D:183:THR:HG22	1:D:185:GLN:HE22	1.83	0.42
1:A:73:GLU:HG2	1:B:159:VAL:HG23	2.01	0.42
1:A:431:LEU:HD13	1:A:448:PHE:CE1	2.55	0.42
1:A:475:VAL:HG13	1:A:504:ILE:HD11	2.00	0.42
1:F:254:LEU:HD21	1:F:577:LEU:HD21	2.01	0.42
1:C:199:ARG:HE	1:C:199:ARG:HB3	1.60	0.42
1:C:403:ARG:NH2	1:F:449:GLU:HG2	2.30	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ILE:HD13	1:C:489:LEU:CD1	2.50	0.42
1:D:159:VAL:HG12	1:D:161:LEU:HD12	2.02	0.42
1:E:559:ASP:OD1	1:E:559:ASP:N	2.51	0.42
1:F:263:LEU:O	1:F:331:GLN:NE2	2.53	0.42
1:B:17:GLU:HG3	1:B:156:LEU:CD1	2.49	0.42
1:B:423:GLY:O	1:B:425:ARG:HG3	2.19	0.42
1:C:29:GLU:OE2	1:C:58:ARG:NH2	2.40	0.42
1:C:210:ARG:CZ	1:D:165:PRO:HG2	2.49	0.42
1:B:401:GLY:HA2	1:B:403:ARG:NH2	2.27	0.42
1:B:468:VAL:HG13	1:B:495:LEU:HD22	2.02	0.42
1:B:466:ASP:OD1	1:B:466:ASP:N	2.51	0.42
1:C:1:MET:SD	1:C:1:MET:N	2.81	0.42
1:C:17:GLU:CB	1:C:127:VAL:HG21	2.49	0.42
1:C:99:ILE:HD12	1:C:116:ALA:CB	2.43	0.42
1:C:181:GLU:CD	1:C:194:SER:HB3	2.45	0.42
1:C:364:TRP:HE3	1:C:412:LEU:HD11	1.85	0.42
1:D:145:GLU:H	1:D:145:GLU:HG3	1.64	0.42
1:D:266:PHE:HB3	1:D:331:GLN:NE2	2.35	0.42
1:D:346:TYR:CE2	1:D:587:ALA:HB1	2.55	0.42
1:A:19:MET:HA	1:A:27:PHE:CE1	2.54	0.42
1:E:268:THR:HG23	1:E:269:HIS:CD2	2.55	0.42
1:E:347:ALA:HB3	1:E:389:VAL:HG22	2.02	0.42
1:F:364:TRP:HE3	1:F:412:LEU:HD11	1.85	0.42
1:F:547:THR:HG22	1:F:560:ASN:ND2	2.35	0.42
1:B:3:ILE:HG23	1:B:29:GLU:CB	2.49	0.42
1:F:250:TRP:CZ3	1:F:573:ARG:HB3	2.55	0.42
1:F:557:LEU:O	1:F:561:LEU:HD13	2.20	0.42
1:B:436:ASP:O	1:B:440:ARG:HB2	2.20	0.42
1:C:170:LEU:CD2	1:C:202:VAL:HG22	2.43	0.41
1:A:48:LEU:HD11	1:A:188:VAL:CG2	2.50	0.41
1:A:256:LYS:HA	1:A:580:GLN:OE1	2.20	0.41
1:B:139:ARG:NH2	1:B:142:SER:OG	2.53	0.41
1:A:489:LEU:HB2	1:A:536:TYR:CZ	2.54	0.41
1:E:435:GLU:HA	1:E:465:ASN:OD1	2.20	0.41
1:F:547:THR:HG22	1:F:560:ASN:HD21	1.85	0.41
1:B:533:LEU:O	1:B:537:LEU:HB2	2.19	0.41
1:C:21:LEU:HB3	1:C:27:PHE:HZ	1.85	0.41
1:C:35:THR:HG21	2:Y:1:A:N1	2.35	0.41
1:D:170:LEU:CD2	1:D:205:VAL:HG11	2.51	0.41
1:D:447:ASP:OD1	1:D:447:ASP:N	2.53	0.41
1:E:251:VAL:HG21	1:E:562:LEU:HD21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:LEU:HD13	1:E:393:LEU:HD21	2.02	0.41
1:E:564:THR:CG2	1:E:571:ILE:HD13	2.50	0.41
1:F:254:LEU:HD11	1:F:577:LEU:HD21	2.03	0.41
1:F:261:CYS:HA	1:F:548:ASP:O	2.19	0.41
1:F:473:GLN:O	1:F:477:LYS:HB2	2.20	0.41
1:C:3:ILE:HD12	1:C:95:ALA:HB3	2.02	0.41
1:C:143:THR:HB	1:C:145:GLU:OE1	2.19	0.41
1:C:211:HIS:ND1	1:C:232:PRO:HD3	2.35	0.41
1:D:101:LEU:CD2	1:D:124:VAL:HG12	2.50	0.41
1:D:292:ILE:HG21	1:D:313:LEU:HA	2.02	0.41
1:A:70:LEU:CD2	1:B:159:VAL:HG11	2.50	0.41
1:E:319:SER:N	3:E:701:ATP:O1B	2.53	0.41
1:F:248:LYS:HD3	1:F:562:LEU:HD11	2.02	0.41
1:F:279:GLU:CB	1:F:330:ALA:HB2	2.50	0.41
1:F:318:GLY:O	1:F:322:LEU:HB2	2.20	0.41
1:F:440:ARG:NH1	1:F:467:ASP:OD1	2.54	0.41
1:C:208:ARG:NH2	1:D:216:TRP:HE1	2.18	0.41
1:C:475:VAL:HG13	1:C:504:ILE:CD1	2.50	0.41
1:D:31:HIS:CE1	1:D:90:ARG:HG3	2.56	0.41
1:B:230:TRP:CZ3	1:B:238:LEU:HD13	2.49	0.41
1:C:298:TRP:CH2	1:C:515:GLN:HB3	2.55	0.41
1:C:473:GLN:O	1:C:477:LYS:HB2	2.21	0.41
1:D:130:GLU:HA	1:D:131:PRO:HD3	1.94	0.41
1:D:475:VAL:HG13	1:D:504:ILE:CD1	2.51	0.41
1:A:131:PRO:HA	1:A:139:ARG:O	2.20	0.41
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.89	0.41
1:A:576:VAL:O	1:A:579:THR:OG1	2.34	0.41
1:E:601:LEU:HD23	1:E:601:LEU:HA	1.86	0.41
1:B:511:TYR:O	1:B:515:GLN:HG3	2.20	0.41
1:D:3:ILE:HG12	1:D:29:GLU:HB2	2.02	0.41
1:D:37:SER:OG	1:D:40:ILE:HD13	2.19	0.41
1:D:129:CYS:HB3	1:D:140:GLU:CD	2.45	0.41
1:D:236:ARG:O	1:D:240:GLU:HG2	2.20	0.41
1:D:271:GLU:O	1:D:275:LYS:HG3	2.20	0.41
1:A:219:ILE:HD12	1:B:216:TRP:HZ3	1.85	0.41
1:A:533:LEU:HD11	1:A:545:LEU:HD21	2.03	0.41
1:E:295:PRO:HA	1:E:296:PRO:HD3	1.96	0.41
1:F:597:LEU:O	1:F:601:LEU:HB2	2.21	0.41
1:B:123:GLU:OE1	1:B:160:ARG:NH2	2.53	0.41
1:C:50:TYR:HA	1:C:53:MET:HG3	2.02	0.41
1:D:206:LEU:HD23	1:D:206:LEU:HA	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:OD1	1:A:405:ARG:HD3	2.21	0.41
1:A:479:SER:O	1:B:502:ARG:NH2	2.54	0.41
1:E:511:TYR:CE1	1:E:563:LEU:HD22	2.56	0.41
1:F:534:ARG:HG3	1:F:568:CYS:HB3	2.03	0.41
1:B:14:VAL:HG11	1:B:102:ALA:HB3	2.03	0.41
1:B:463:GLY:C	1:B:464:GLU:HG3	2.46	0.41
1:C:99:ILE:HG23	1:C:112:MET:HE3	2.02	0.41
1:C:149:GLN:HE21	1:C:149:GLN:HB3	1.63	0.41
1:C:533:LEU:CD1	1:C:543:VAL:HG11	2.50	0.41
1:D:67:PHE:CE1	1:D:79:PHE:HB2	2.55	0.41
1:D:441:ALA:O	1:D:478:LEU:HD11	2.21	0.41
1:A:8:VAL:HG11	1:A:15:VAL:HG23	2.02	0.41
1:A:83:LEU:HD11	1:A:112:MET:CE	2.37	0.41
1:F:386:ARG:O	1:F:600:ARG:NH1	2.54	0.41
1:F:471:ILE:HB	1:F:495:LEU:HD21	2.03	0.41
1:B:134:GLY:HA3	1:B:139:ARG:CG	2.51	0.41
1:B:221:GLU:H	1:B:221:GLU:HG3	1.73	0.41
1:B:273:LEU:HD21	1:B:316:ASN:HB3	2.01	0.41
1:B:294:LEU:HD23	1:B:313:LEU:HD21	2.03	0.41
1:B:356:TYR:HB2	1:B:366:VAL:HG11	2.02	0.41
1:B:581:VAL:HG13	1:B:598:TRP:CH2	2.56	0.41
1:C:192:ARG:HB3	1:C:192:ARG:HH11	1.85	0.41
1:A:113:GLN:HE21	1:B:110:ALA:HB1	1.86	0.41
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.03	0.41
1:A:218:GLY:C	1:A:220:SER:H	2.28	0.41
1:A:277:ARG:CG	1:A:321:LEU:HD11	2.51	0.41
1:A:397:ARG:HG2	1:A:432:ALA:O	2.21	0.41
1:F:256:LYS:HA	1:F:580:GLN:OE1	2.21	0.41
1:B:302:GLU:HB2	1:B:303:GLU:OE1	2.20	0.41
1:C:298:TRP:CG	1:C:299:PRO:HA	2.56	0.40
1:A:311:MET:HE3	3:A:701:ATP:H2'	2.03	0.40
1:E:251:VAL:O	1:E:256:LYS:NZ	2.54	0.40
1:B:124:VAL:O	1:B:161:LEU:N	2.52	0.40
1:C:216:TRP:HE1	1:D:208:ARG:HH22	1.69	0.40
1:C:475:VAL:HG13	1:C:504:ILE:HD11	2.03	0.40
1:D:13:ALA:HB3	2:Y:5:A:N6	2.35	0.40
1:D:183:THR:CG2	1:D:185:GLN:HE22	2.34	0.40
1:D:507:GLU:HB3	1:D:546:ASN:HD21	1.87	0.40
1:A:71:ARG:O	1:A:72:SER:HB3	2.21	0.40
1:A:447:ASP:O	1:A:450:PRO:HD2	2.21	0.40
1:A:467:ASP:OD1	1:A:467:ASP:N	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:PRO:O	1:F:515:GLN:NE2	2.54	0.40
1:C:99:ILE:CG2	1:C:112:MET:HE3	2.51	0.40
1:A:130:GLU:OE2	1:A:132:ARG:HB2	2.20	0.40
1:E:350:ARG:NH2	1:E:459:THR:HG21	2.36	0.40
1:E:475:VAL:HG13	1:E:504:ILE:CD1	2.51	0.40
1:B:178:PHE:CE1	1:B:197:ARG:HG2	2.56	0.40
1:C:47:LEU:HD22	1:C:51:PHE:CZ	2.55	0.40
1:D:36:ALA:HB2	1:D:64:VAL:O	2.21	0.40
1:D:75:ASP:HA	1:D:78:LEU:HD12	2.03	0.40
1:D:78:LEU:O	1:D:82:VAL:HG23	2.21	0.40
1:D:81:GLU:O	1:D:85:ARG:HG3	2.22	0.40
1:A:3:ILE:CD1	1:A:95:ALA:HB1	2.51	0.40
1:A:254:LEU:CD1	1:A:605:PRO:HD2	2.51	0.40
1:F:254:LEU:HD23	1:F:255:PRO:HD2	2.03	0.40
1:C:114:ARG:HD3	1:D:113:GLN:NE2	2.37	0.40
1:C:208:ARG:O	1:C:212:ILE:HG13	2.21	0.40
1:C:497:ARG:HH22	1:D:455:GLY:HA3	1.87	0.40
1:D:1:MET:CE	1:D:29:GLU:HG3	2.52	0.40
1:D:49:ARG:HA	1:D:52:GLU:OE1	2.21	0.40
1:D:449:GLU:HB3	1:D:450:PRO:HD3	2.03	0.40
1:E:403:ARG:O	1:E:406:ILE:HG22	2.22	0.40
1:B:1:MET:HB2	1:B:28:ASP:HB2	2.04	0.40
1:B:81:GLU:OE1	1:B:198:LEU:HB3	2.21	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 PDB entries followed by that with respect to all EM entries.

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	608/631 (96%)	573 (94%)	35 (6%)	0	100	100
1	B	605/631 (96%)	580 (96%)	23 (4%)	2 (0%)	36	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	587/631 (93%)	539 (92%)	47 (8%)	1 (0%)	43	65
1	D	608/631 (96%)	582 (96%)	25 (4%)	1 (0%)	43	65
1	E	386/631 (61%)	367 (95%)	19 (5%)	0	100	100
1	F	390/631 (62%)	368 (94%)	20 (5%)	2 (0%)	24	49
All	All	3184/3786 (84%)	3009 (94%)	169 (5%)	6 (0%)	44	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	36	ALA
1	B	464	GLU
1	F	464	GLU
1	D	68	GLU
1	F	548	ASP
1	B	524	GLU

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 PDB entries followed by that with respect to all EM entries.

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	499/517 (96%)	485 (97%)	14 (3%)	38	63
1	B	496/517 (96%)	481 (97%)	15 (3%)	36	61
1	C	487/517 (94%)	469 (96%)	18 (4%)	30	55
1	D	498/517 (96%)	484 (97%)	14 (3%)	38	63
1	E	313/517 (60%)	307 (98%)	6 (2%)	50	71
1	F	315/517 (61%)	311 (99%)	4 (1%)	61	77
All	All	2608/3102 (84%)	2537 (97%)	71 (3%)	40	64

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	28	ASP
1	C	35	THR
1	C	37	SER
1	C	71	ARG
1	C	81	GLU
1	C	136	GLN
1	C	149	GLN
1	C	153	THR
1	C	169	GLN
1	C	198	LEU
1	C	216	TRP
1	C	302	GLU
1	C	422	ASN
1	C	431	LEU
1	C	461	HIS
1	C	529	GLU
1	C	601	LEU
1	D	6	CYS
1	D	27	PHE
1	D	40	ILE
1	D	83	LEU
1	D	101	LEU
1	D	183	THR
1	D	192	ARG
1	D	303	GLU
1	D	399	GLU
1	D	461	HIS
1	D	478	LEU
1	D	544	THR
1	D	575	GLU
1	D	608	THR
1	A	29	GLU
1	A	34	THR
1	A	37	SER
1	A	70	LEU
1	A	87	LEU
1	A	89	GLN
1	A	96	HIS
1	A	101	LEU
1	A	112	MET
1	A	153	THR
1	A	159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	161	LEU
1	A	198	LEU
1	A	530	THR
1	E	222	LEU
1	E	230	TRP
1	E	459	THR
1	E	461	HIS
1	E	572	THR
1	E	600	ARG
1	F	459	THR
1	F	461	HIS
1	F	530	THR
1	F	572	THR
1	B	17	GLU
1	B	32	VAL
1	B	45	GLU
1	B	80	GLU
1	B	96	HIS
1	B	122	CYS
1	B	159	VAL
1	B	219	ILE
1	B	313	LEU
1	B	340	LEU
1	B	422	ASN
1	B	436	ASP
1	B	459	THR
1	B	550	LEU
1	B	601	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	25	GLN
1	C	76	HIS
1	C	89	GLN
1	C	252	GLN
1	C	278	GLN
1	C	461	HIS
1	C	513	ASN
1	D	31	HIS
1	D	76	HIS
1	D	93	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	96	HIS
1	D	136	GLN
1	D	185	GLN
1	D	278	GLN
1	D	390	ASN
1	D	485	HIS
1	D	546	ASN
1	D	554	GLN
1	A	54	HIS
1	A	126	HIS
1	A	390	ASN
1	A	485	HIS
1	A	513	ASN
1	E	269	HIS
1	E	452	HIS
1	E	485	HIS
1	E	513	ASN
1	F	513	ASN
1	F	560	ASN
1	B	20	GLN
1	B	46	GLN
1	B	316	ASN
1	B	390	ASN
1	B	473	GLN
1	B	585	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	5/6 (83%)	5 (100%)	0
2	Y	5/6 (83%)	2 (40%)	0
All	All	10/12 (83%)	7 (70%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	2	A
2	X	3	A
2	X	4	A
2	X	5	A
2	X	6	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	2	A
2	Y	5	A

There are no RNA pucker outliers to report.

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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	F	701	5	29,33,33	0.34	0	44,52,52	0.83	1 (2%)
3	ATP	B	701	5	29,33,33	0.32	0	44,52,52	0.77	1 (2%)
3	ATP	C	701	5	29,33,33	0.47	0	44,52,52	0.56	0
3	ATP	E	701	5	29,33,33	0.33	0	44,52,52	0.79	1 (2%)
3	ATP	A	701	5	29,33,33	0.34	0	44,52,52	0.85	1 (2%)
3	ATP	D	701	5	29,33,33	0.32	0	44,52,52	0.74	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	F	701	5	-	4/22/38/38	0/3/3/3
3	ATP	B	701	5	-	1/22/38/38	0/3/3/3
3	ATP	C	701	5	-	2/22/38/38	0/3/3/3
3	ATP	E	701	5	-	2/22/38/38	0/3/3/3
3	ATP	A	701	5	-	2/22/38/38	0/3/3/3
3	ATP	D	701	5	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	701	ATP	PB-O3B-PG	2.10	140.03	132.83
3	B	701	ATP	PB-O3B-PG	2.05	139.87	132.83
3	A	701	ATP	PB-O3B-PG	2.02	139.76	132.83
3	D	701	ATP	PB-O3B-PG	2.02	139.74	132.83
3	F	701	ATP	PB-O3B-PG	2.01	139.74	132.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

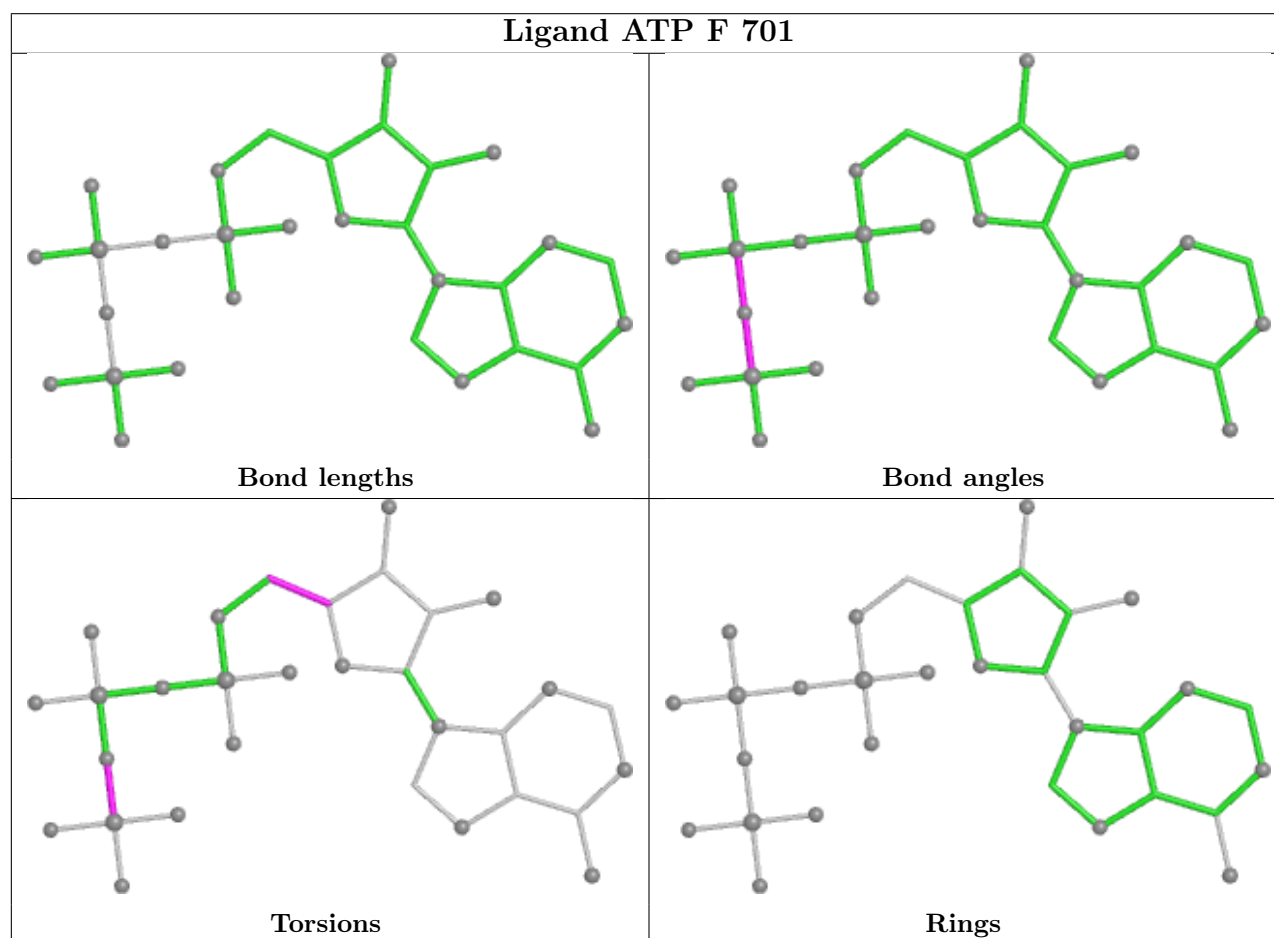
Mol	Chain	Res	Type	Atoms
3	A	701	ATP	PB-O3B-PG-O2G
3	E	701	ATP	PB-O3B-PG-O3G
3	F	701	ATP	PB-O3B-PG-O2G
3	D	701	ATP	O4'-C4'-C5'-O5'
3	F	701	ATP	O4'-C4'-C5'-O5'
3	F	701	ATP	C3'-C4'-C5'-O5'
3	D	701	ATP	PB-O3B-PG-O1G
3	C	701	ATP	PA-O3A-PB-O2B
3	D	701	ATP	PB-O3A-PA-O1A
3	E	701	ATP	PB-O3A-PA-O1A
3	D	701	ATP	PG-O3B-PB-O2B
3	D	701	ATP	PB-O3B-PG-O2G
3	D	701	ATP	PB-O3B-PG-O3G
3	A	701	ATP	PB-O3B-PG-O3G
3	F	701	ATP	PB-O3B-PG-O3G
3	C	701	ATP	PA-O3A-PB-O1B
3	B	701	ATP	C5'-O5'-PA-O1A
3	D	701	ATP	C3'-C4'-C5'-O5'

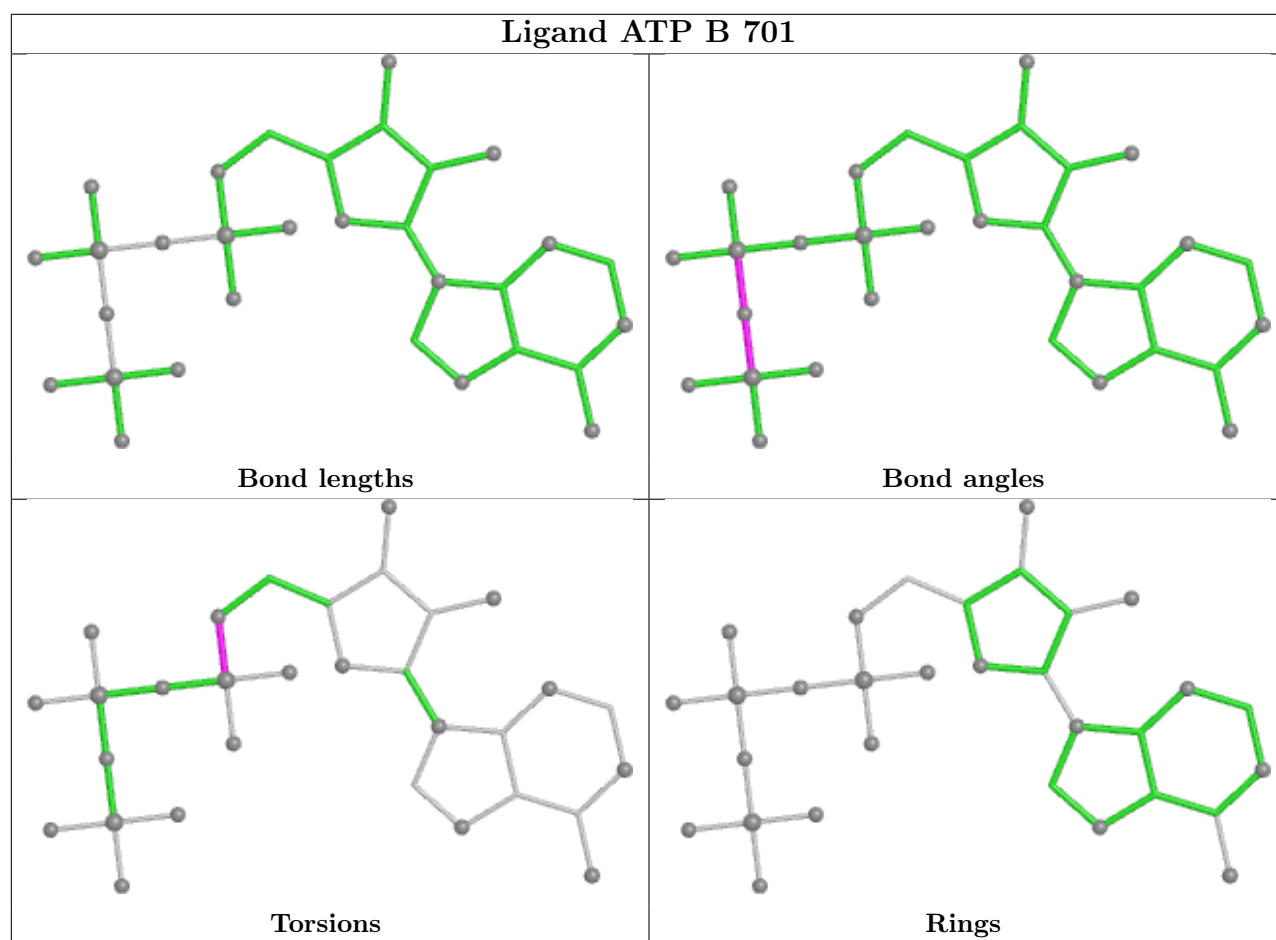
There are no ring outliers.

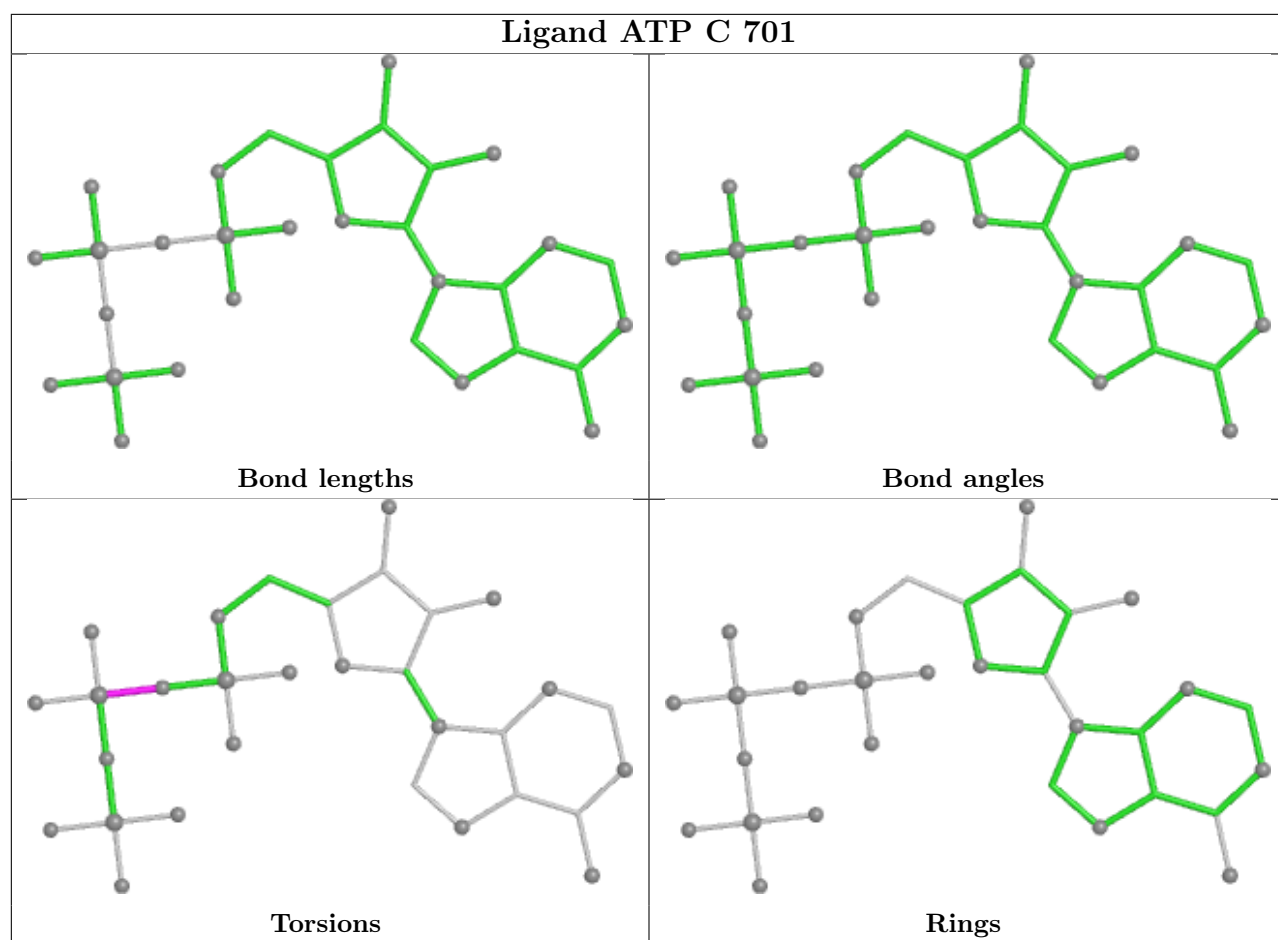
4 monomers are involved in 6 short contacts:

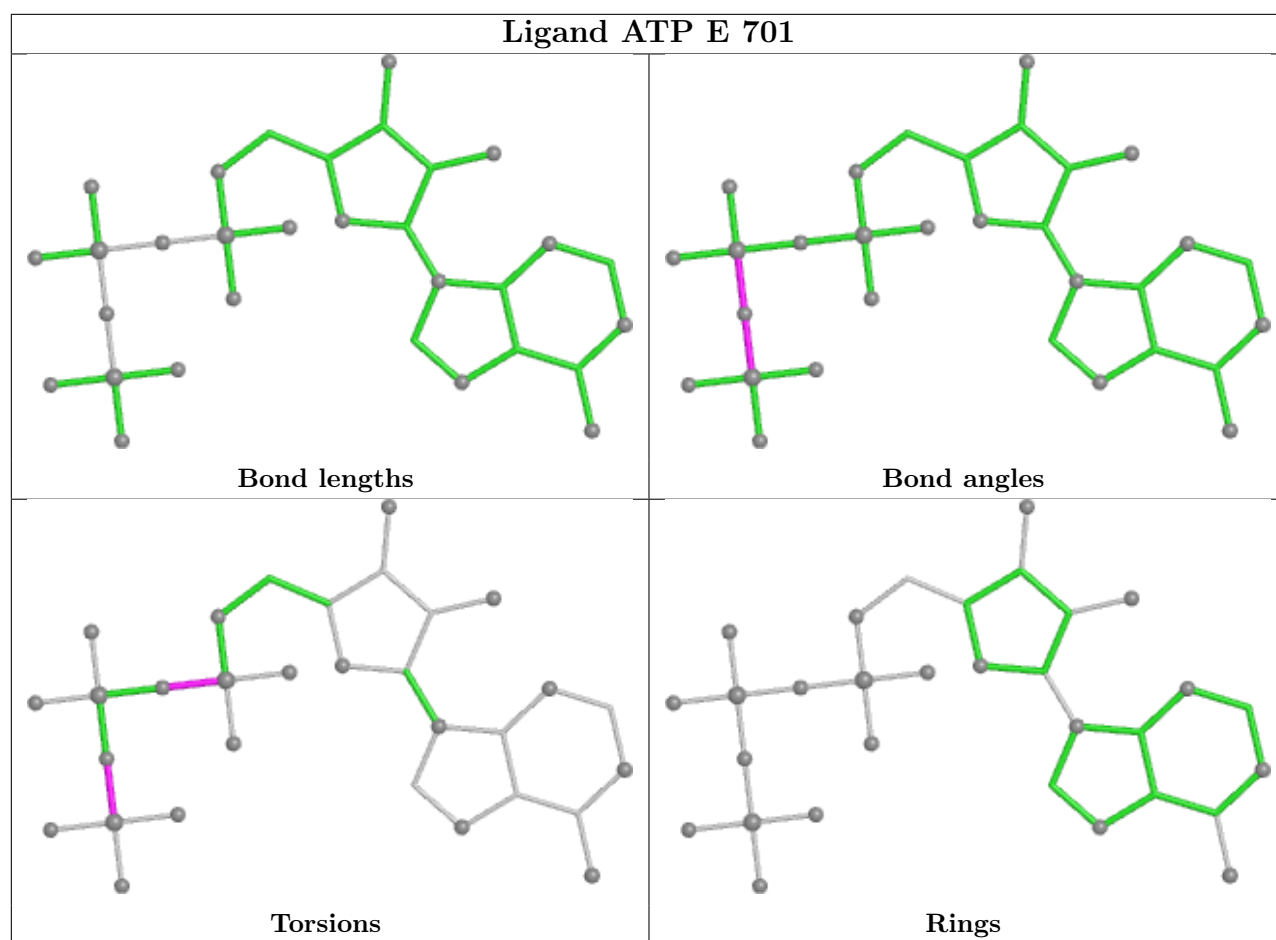
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	701	ATP	1	0
3	C	701	ATP	1	0
3	E	701	ATP	2	0
3	A	701	ATP	2	0

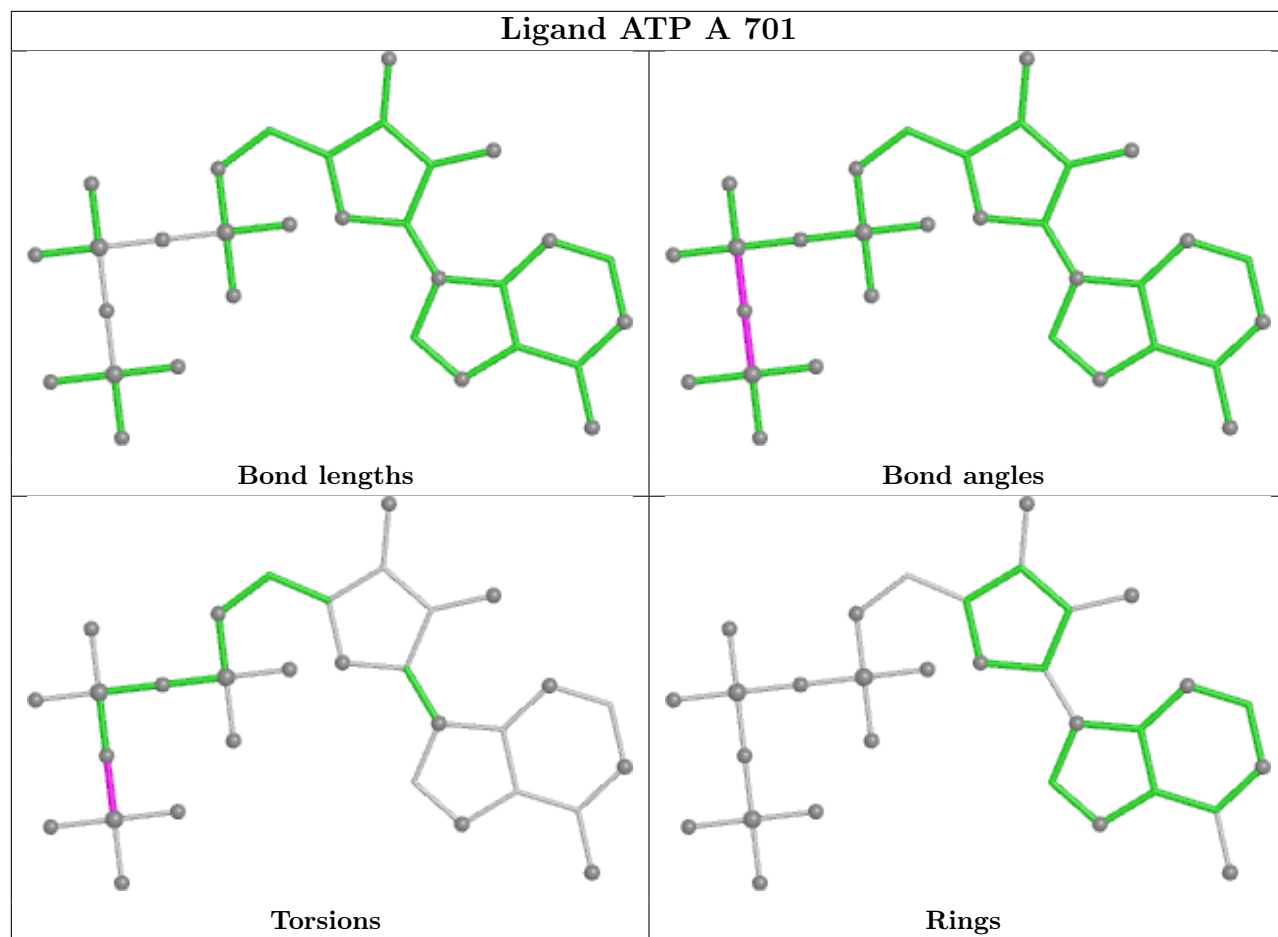
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

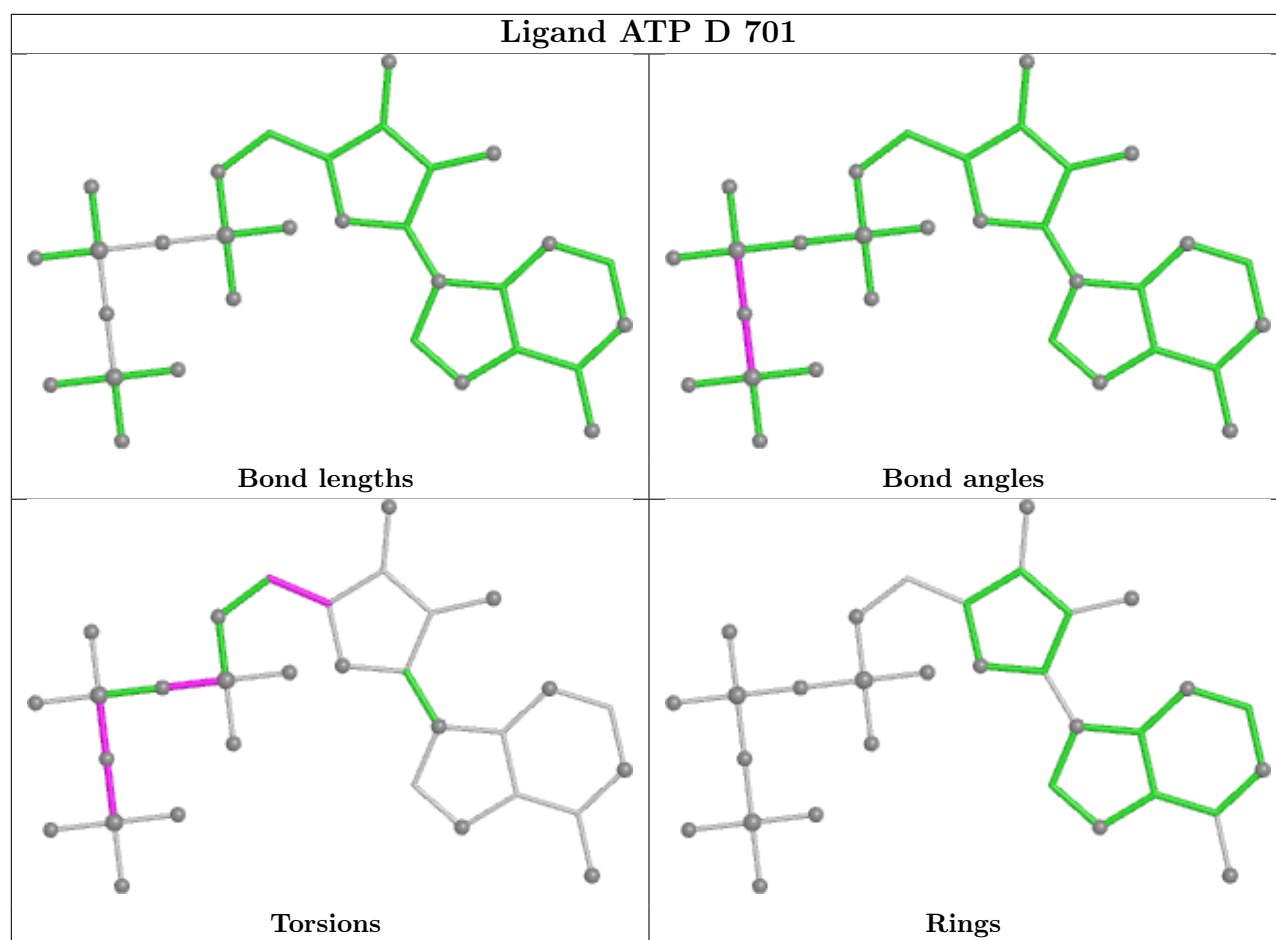












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

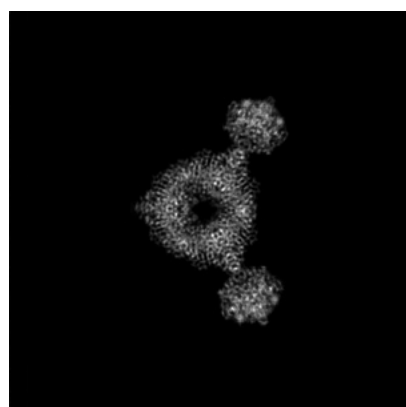
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65540. These allow visual inspection of the internal detail of the map and identification of artifacts.

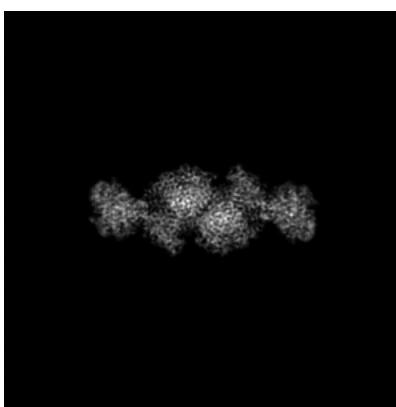
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

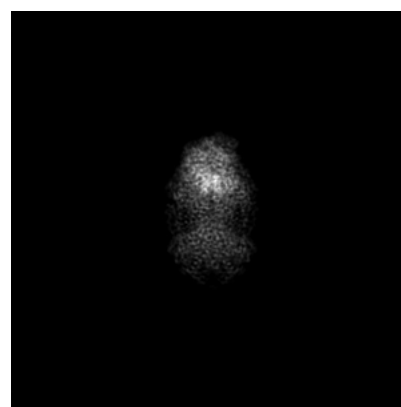
6.1.1 Primary map



X



Y

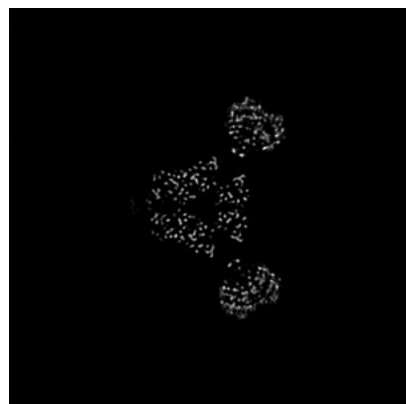


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

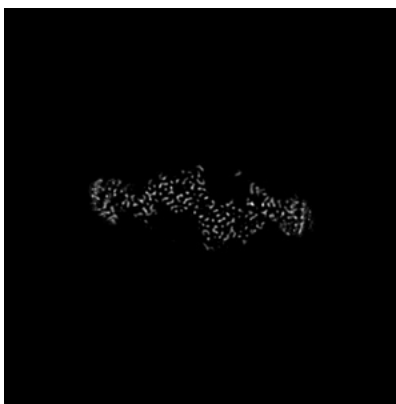
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 196



Y Index: 220

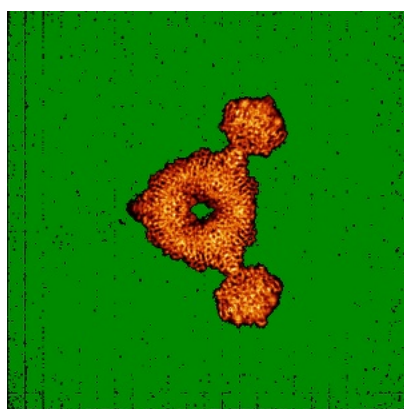


Z Index: 162

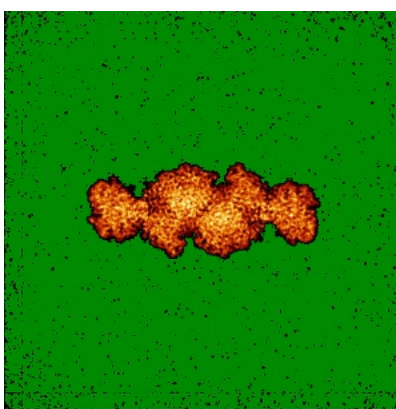
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

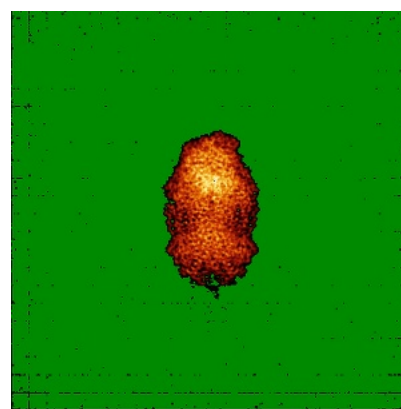
6.4.1 Primary map



X



Y

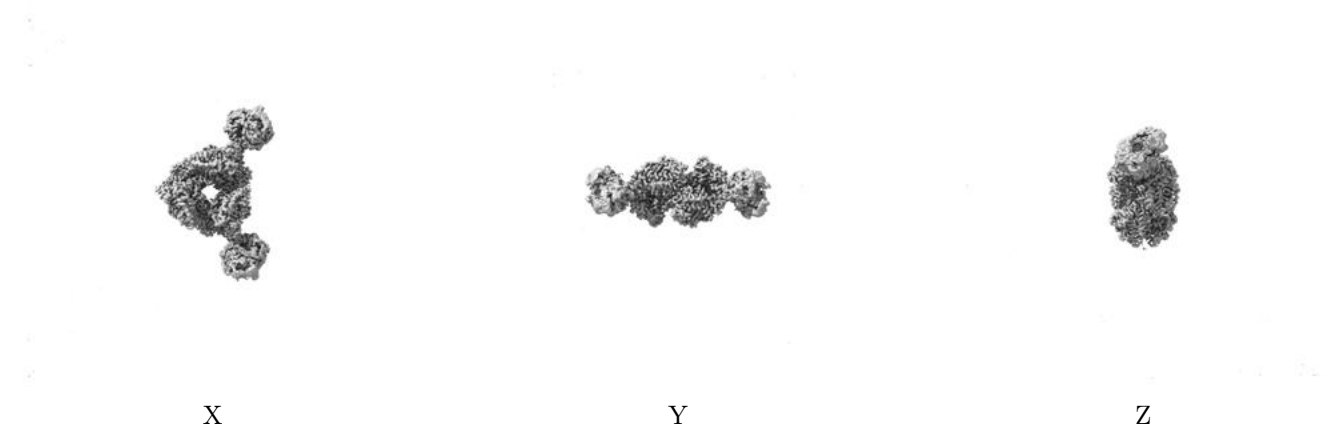


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

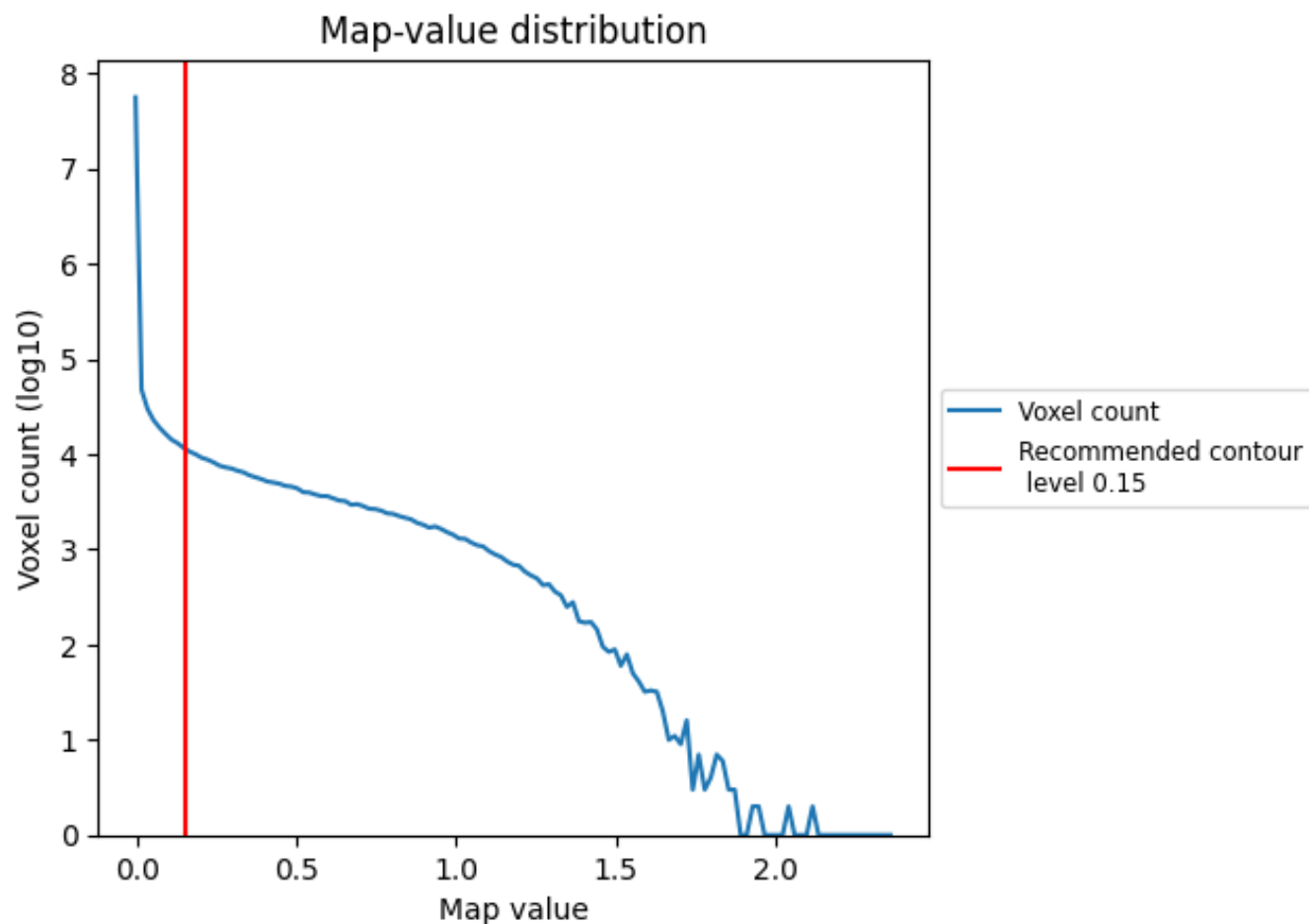
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

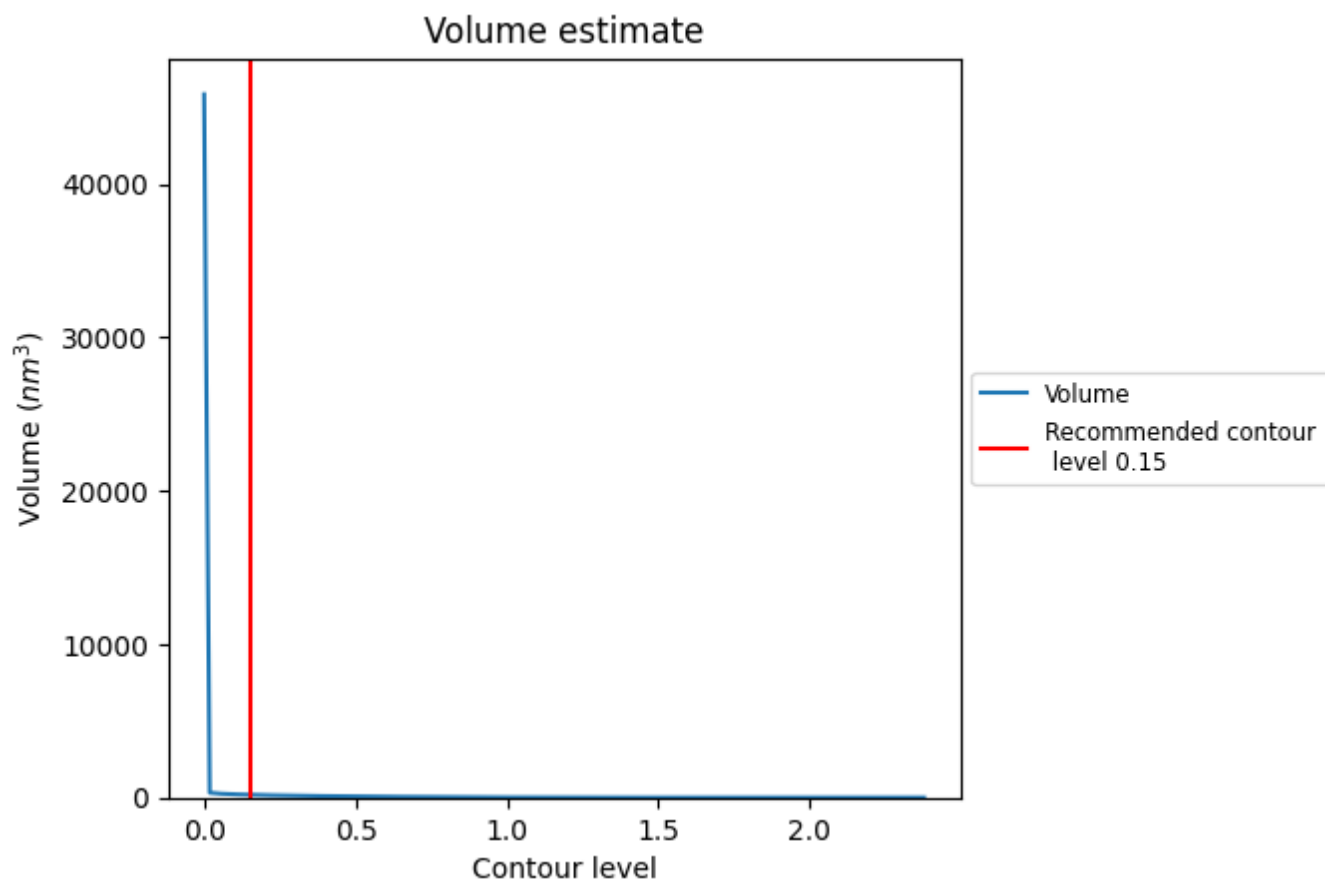
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

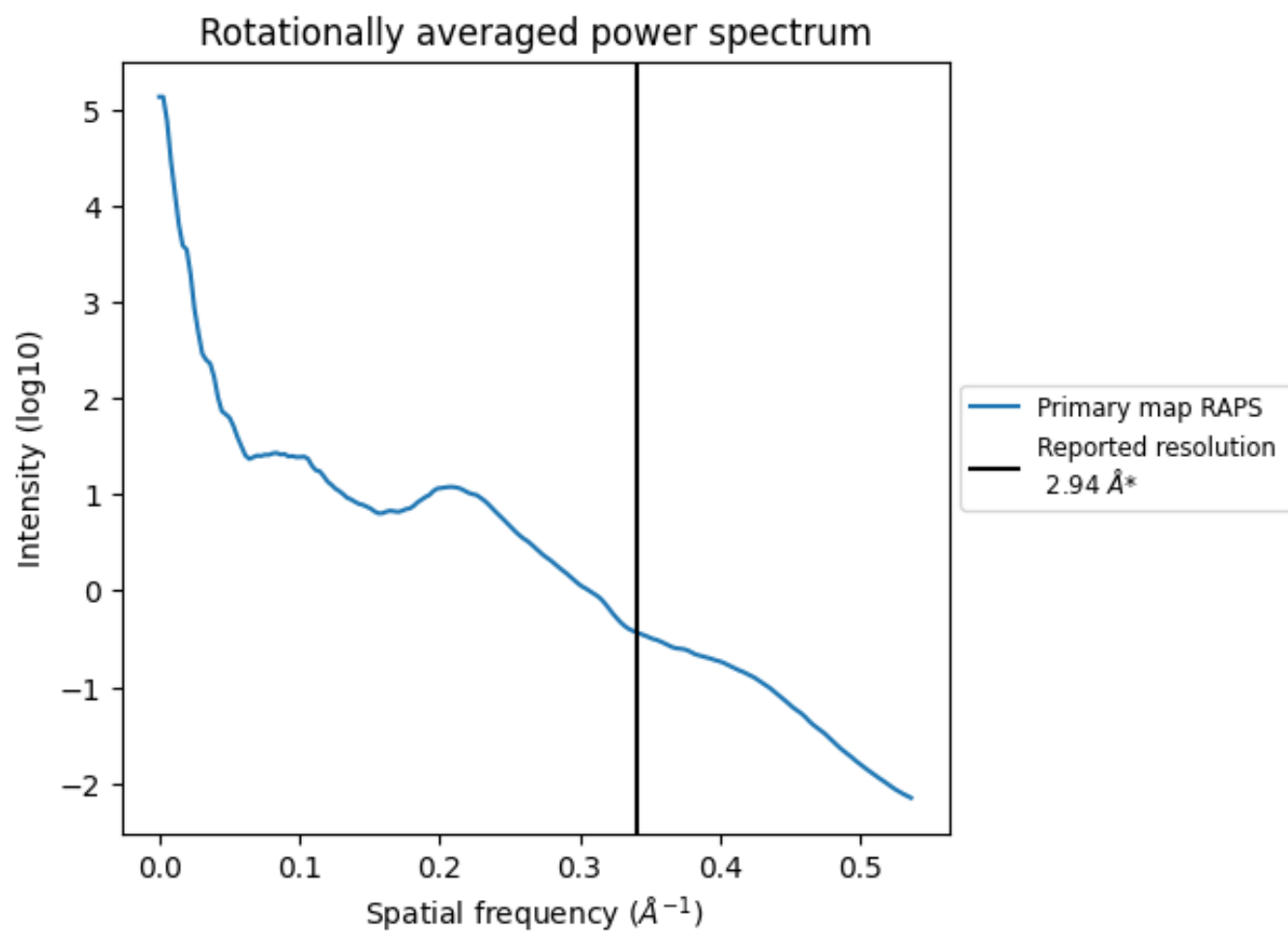
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

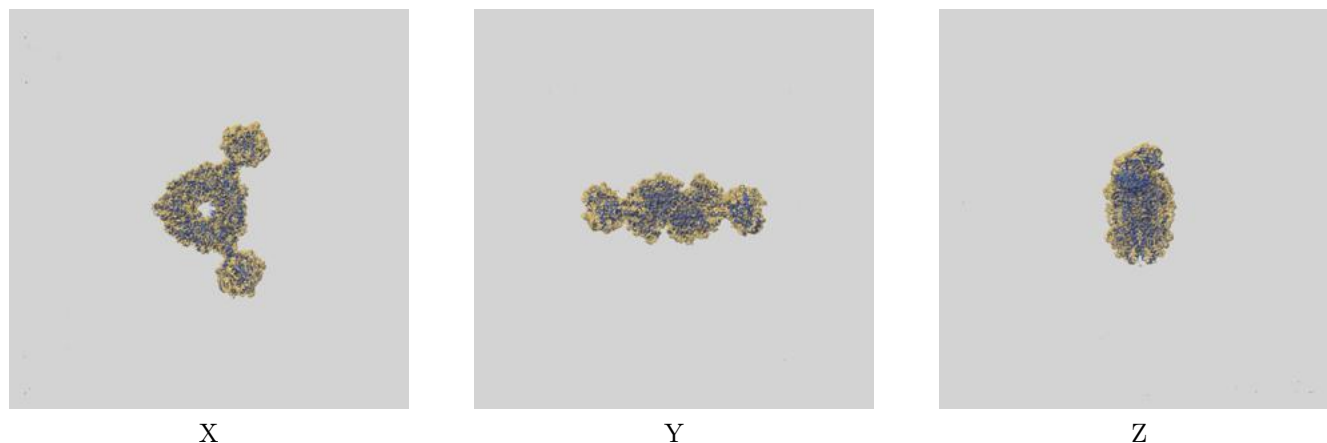
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

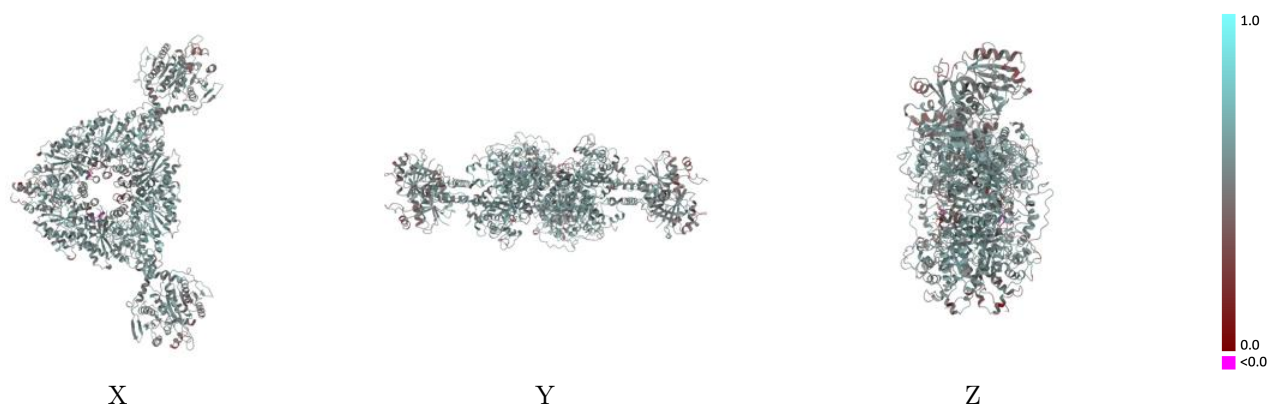
This section contains information regarding the fit between EMDB map EMD-65540 and PDB model 9W1H. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



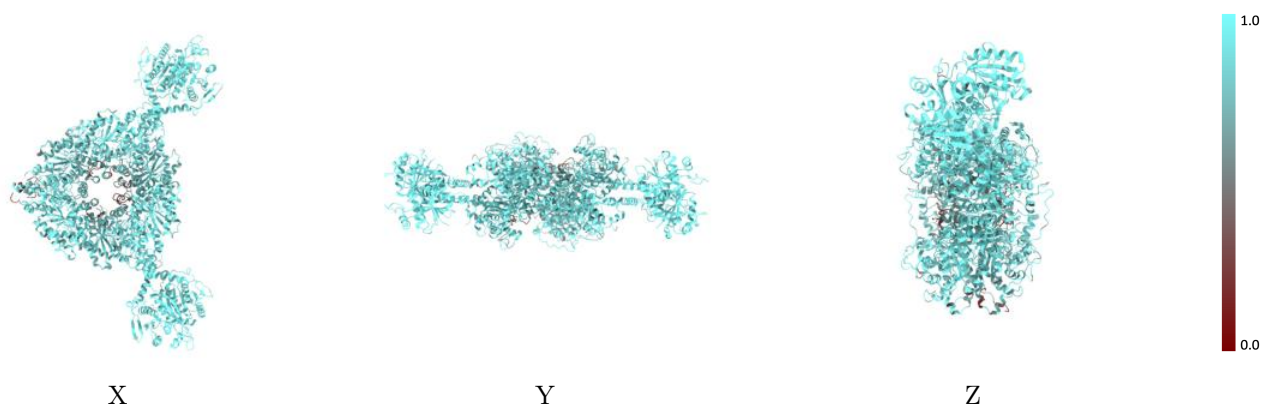
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



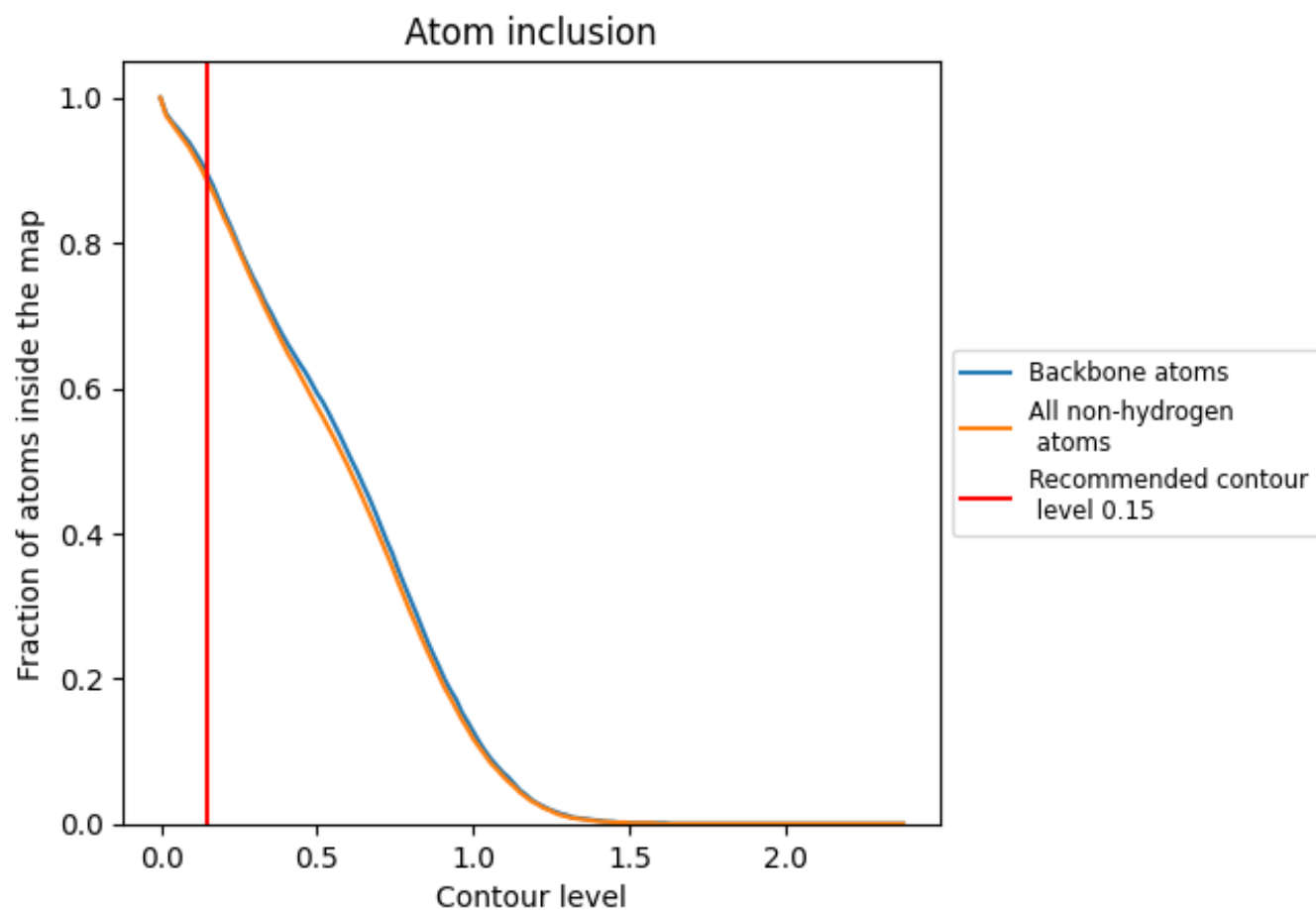
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8830	<div><div></div></div> 0.5320
A	<div><div></div></div> 0.8910	<div><div></div></div> 0.5330
B	<div><div></div></div> 0.8910	<div><div></div></div> 0.5220
C	<div><div></div></div> 0.9110	<div><div></div></div> 0.5380
D	<div><div></div></div> 0.8980	<div><div></div></div> 0.5420
E	<div><div></div></div> 0.8620	<div><div></div></div> 0.5320
F	<div><div></div></div> 0.8570	<div><div></div></div> 0.5270
X	<div><div></div></div> 0.9550	<div><div></div></div> 0.4740
Y	<div><div></div></div> 0.9920	<div><div></div></div> 0.5200

1.0

0.0

<0.0