



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:16 PM GMT

PDB ID : 4EAH
Title : Crystal structure of the formin homology 2 domain of FMNL3 bound to actin
Authors : Thompson, M.E.; Heimsath, E.G.; Gauvin, T.J.; Higgs, H.N.; Kull, F.J.
Deposited on : 2012-03-22
Resolution : 3.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

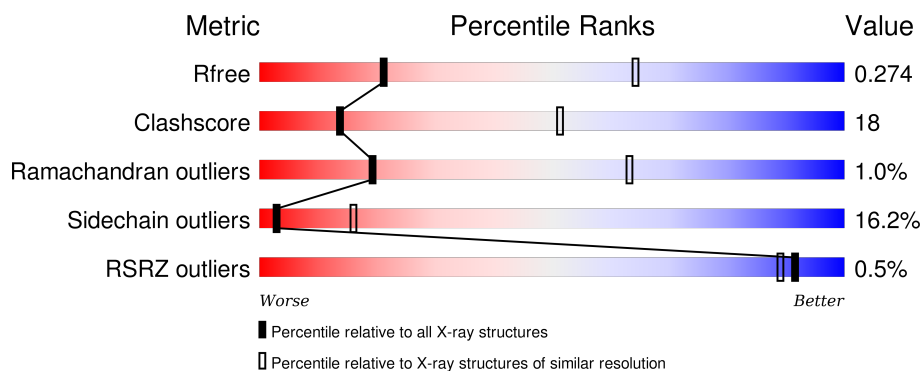
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	D	377	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>33%</div> <div>6%</div> <div>6%</div> </div> </div>
1	F	377	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>6%</div> <div>6%</div> </div> </div>
1	G	377	<div> <div></div> <div> <div></div> <div>54%</div> <div>35%</div> <div>5%</div> <div>6%</div> </div> </div>
1	H	377	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>37%</div> <div>5%</div> <div>6%</div> </div> </div>
2	A	402	<div> <div></div> <div> <div></div> <div>51%</div> <div>30%</div> <div>7%</div> <div>11%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	402	
2	C	402	
2	E	402	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	B	1001	-	-	X	-
3	ACT	D	401	-	-	X	-
3	ACT	E	1001	-	-	-	X
3	ACT	F	401	-	-	-	X
3	ACT	G	401	-	-	X	-
3	ACT	H	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22892 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	356	Total	C	N	O	S	121	0	0
			2785	1766	468	533	18			
1	H	356	Total	C	N	O	S	123	0	0
			2785	1766	468	533	18			
1	G	356	Total	C	N	O	S	132	0	0
			2785	1766	468	533	18			
1	F	356	Total	C	N	O	S	65	0	0
			2785	1766	468	533	18			

- Molecule 2 is a protein called Formin-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	357	Total	C	N	O	S	265	0	0
			2895	1848	502	533	12			
2	E	357	Total	C	N	O	S	272	0	0
			2895	1848	502	533	12			
2	C	357	Total	C	N	O	S	252	0	0
			2895	1848	502	533	12			
2	B	357	Total	C	N	O	S	260	0	0
			2895	1848	502	533	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
A	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4
E	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
E	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4
C	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
C	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4
B	553	GLY	-	EXPRESSION TAG	UNP Q6ZPF4
B	554	SER	-	EXPRESSION TAG	UNP Q6ZPF4

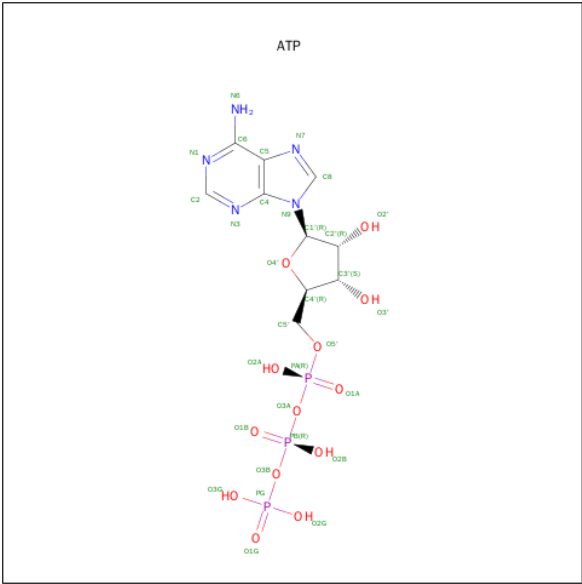
- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

C₁₀H₁₆N₅O₁₃P₃).

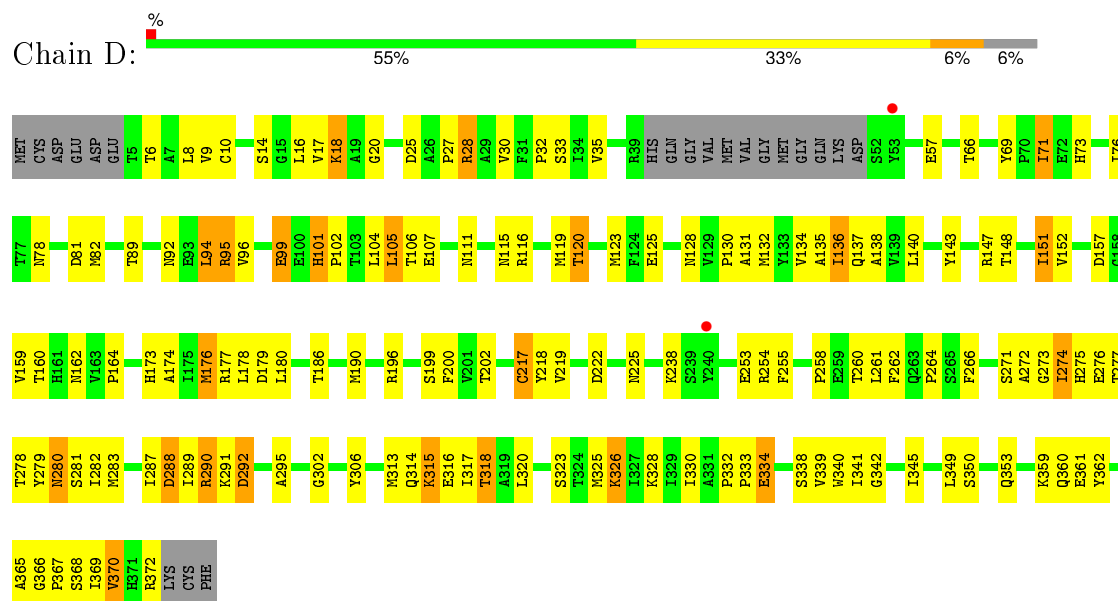


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

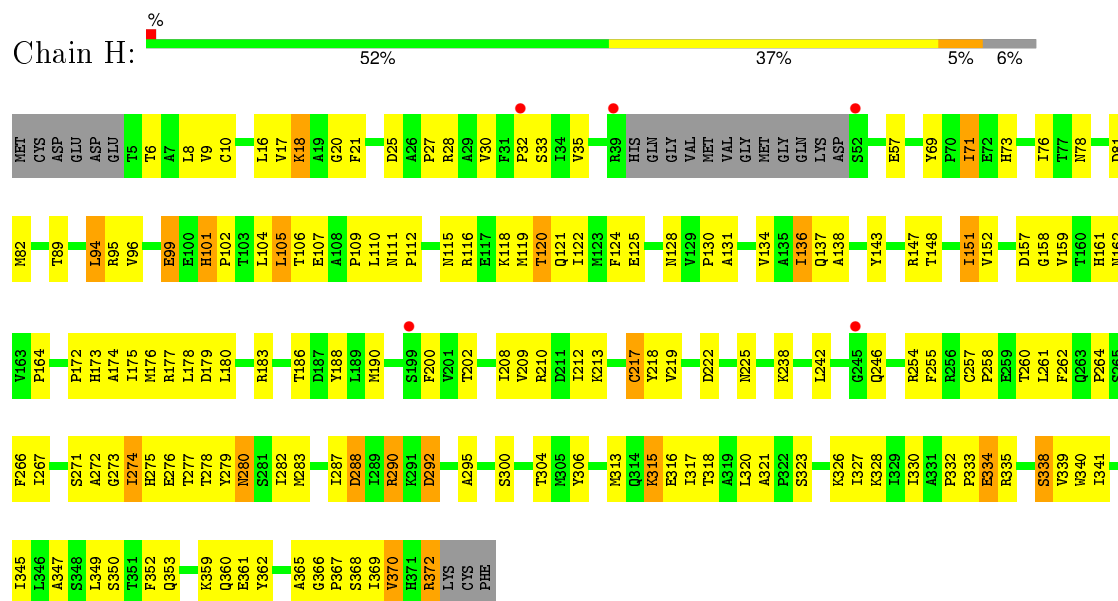
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

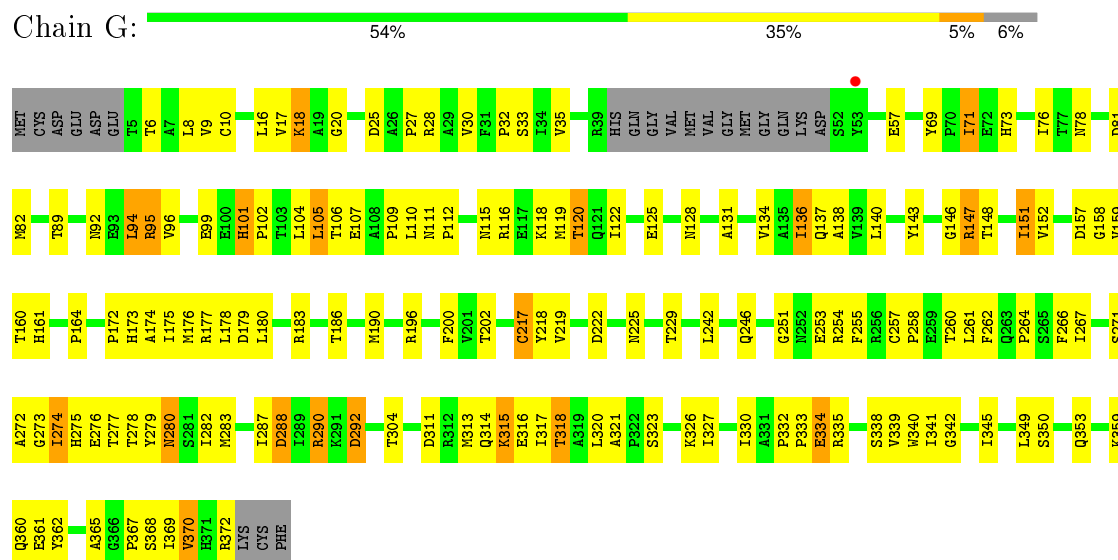
• Molecule 1: Actin, alpha skeletal muscle



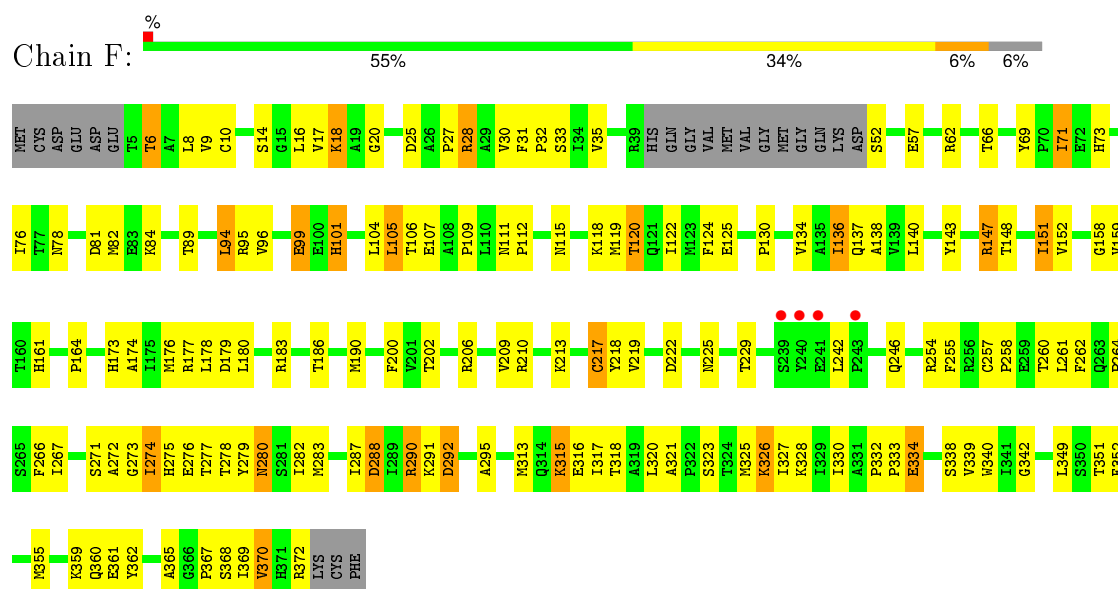
• Molecule 1: Actin, alpha skeletal muscle



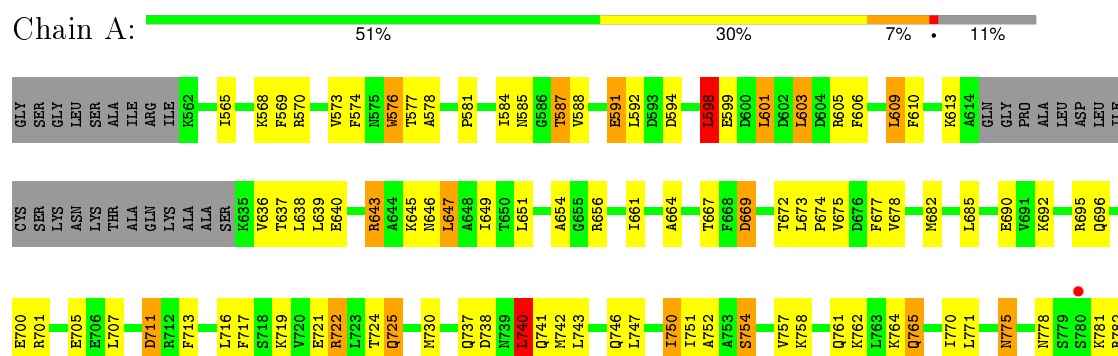
• Molecule 1: Actin, alpha skeletal muscle

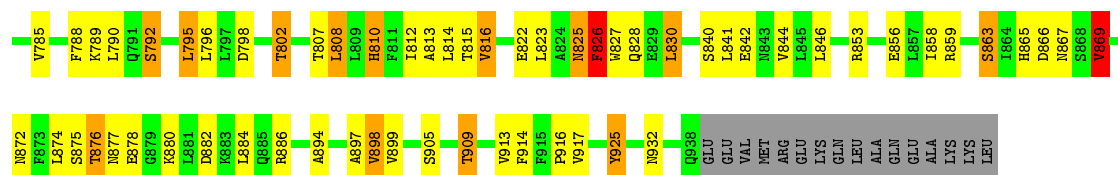


• Molecule 1: Actin, alpha skeletal muscle



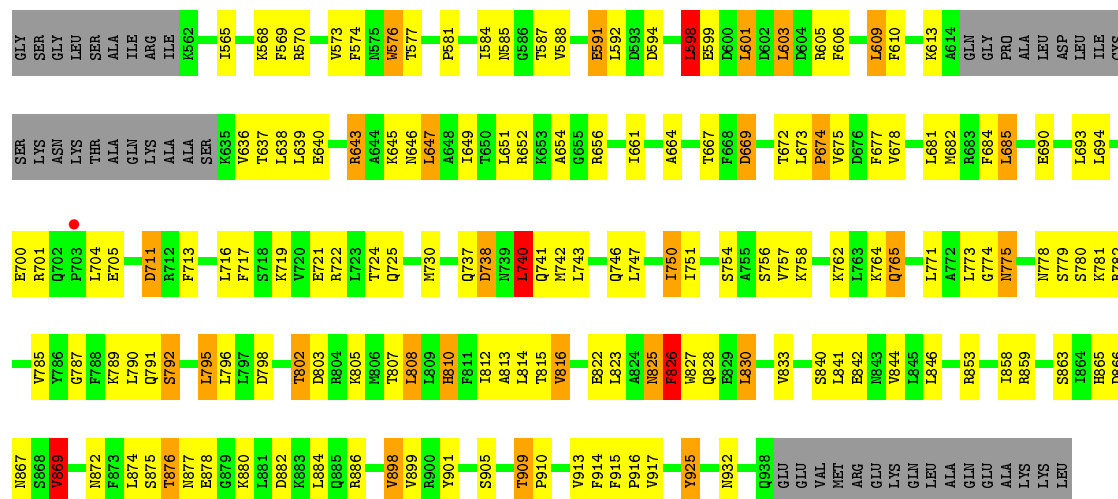
• Molecule 2: Formin-like protein 3





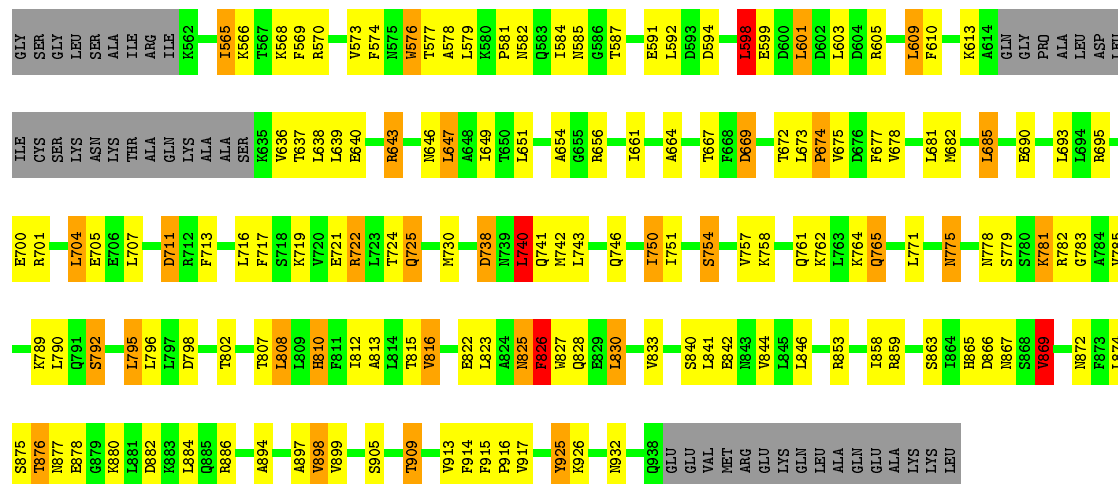
• Molecule 2: Formin-like protein 3

Chain E: 49% 32% 7% 11%



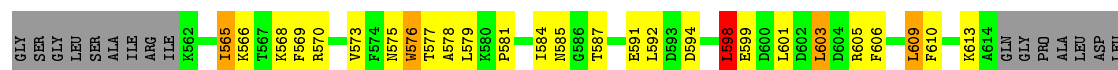
• Molecule 2: Formin-like protein 3

Chain C: 51% 29% 7% 11%



• Molecule 2: Formin-like protein 3

Chain B: 50% 30% 8% 11%



ILE	S868	V869	N872	F873	L874	S875	T876	N877	K880	L881	D882	K883	L884	R886	A894	A897	V898	V899	S905	T909	V913	F914	F915	F916	Y925	N932	Q938	GLU	GLU	VAL	MET	ARG	GLU	LYS	GLN	LEU	ALA	GLU	ALA	LYS	LYS	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
	V785	K789	L790	Q791	S792	L795	L796	L797	D798	T802	T807	L808	L809	H810	F811	I812	A813	L814	T815	V816	E822	L823	N824	N825	F826	H827	Q828	E829	L830	V833	S840	L841	E842	N843	V844	L845	L846	E850	R853	E856	L857	I858	R859	S863	L864	H865	D866	N867																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
	L693	L694	R695	E700	R701	E705	E706	L707	D711	R712	F713	L716	F717	S718	K719	V720	E721	R722	L723	T724	Q725	Q737	D738	T739	L740	Q741	N742	L743	Q746	I750	I751	S754	V757	K758	Q761	K762	L763	F677	V678	L681	H682	L685	H686	T687	N778	S779	L780	K781																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.98Å 126.05Å 129.62Å 90.00° 93.17° 90.00°	Depositor
Resolution (Å)	19.82 – 3.40 19.82 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.82-3.40) 99.8 (19.82-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.230 , 0.277 0.224 , 0.274	Depositor DCC
R_{free} test set	2892 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.6	EDS
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 55418 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22892	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	D	0.51	0/2845	0.70	0/3858
1	F	0.48	0/2845	0.69	0/3858
1	G	0.48	0/2845	0.70	0/3858
1	H	0.48	0/2845	0.70	0/3858
2	A	0.48	0/2942	0.70	1/3956 (0.0%)
2	B	0.49	0/2942	0.69	1/3956 (0.0%)
2	C	0.49	0/2942	0.70	1/3956 (0.0%)
2	E	0.49	0/2942	0.70	1/3956 (0.0%)
All	All	0.49	0/23148	0.70	4/31256 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	740	LEU	CA-CB-CG	5.37	127.64	115.30
2	C	740	LEU	CA-CB-CG	5.25	127.37	115.30
2	A	740	LEU	CA-CB-CG	5.15	127.14	115.30
2	B	740	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2785	0	2758	100	1
1	F	2785	0	2758	97	1
1	G	2785	0	2758	105	0
1	H	2785	0	2758	111	0
2	A	2895	0	2971	101	0
2	B	2895	0	2971	104	0
2	C	2895	0	2971	99	0
2	E	2895	0	2971	105	0
3	A	12	0	9	1	0
3	B	4	0	3	2	0
3	C	8	0	6	2	0
3	D	4	0	3	2	0
3	E	4	0	3	1	0
3	F	8	0	6	1	0
3	G	4	0	3	2	0
3	H	4	0	3	2	0
4	D	31	0	12	5	0
4	F	31	0	12	1	0
4	G	31	0	12	2	0
4	H	31	0	12	2	0
All	All	22892	0	23000	776	1

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 (776) 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:H:147:ARG:HH12	1:H:330:ILE:HG12	1.29	0.94
1:H:261:LEU:HB3	1:H:274:ILE:HD11	1.54	0.90
1:D:261:LEU:HB3	1:D:274:ILE:HD11	1.55	0.89
1:D:147:ARG:HH12	1:D:330:ILE:HG12	1.36	0.88
1:G:261:LEU:HB3	1:G:274:ILE:HD11	1.55	0.88
1:G:137:GLN:NE2	4:G:402:ATP:O3G	2.08	0.87
1:G:147:ARG:HH12	1:G:330:ILE:HG12	1.39	0.86
1:F:261:LEU:HB3	1:F:274:ILE:HD11	1.58	0.85
1:F:147:ARG:HH12	1:F:330:ILE:HG12	1.41	0.85
1:H:137:GLN:NE2	4:H:402:ATP:O3G	2.11	0.83
2:B:746:GLN:HE22	1:H:323:SER:HB3	1.44	0.82
2:A:778:ASN:ND2	3:A:1003:ACT:O	2.14	0.81
2:A:758:LYS:HB2	2:A:898:VAL:HG13	1.62	0.81
2:E:789:LYS:O	2:E:792:SER:OG	1.97	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:789:LYS:O	2:C:792:SER:OG	2.00	0.79
2:B:807:THR:HG23	2:B:810:HIS:H	1.48	0.79
2:E:758:LYS:HB2	2:E:898:VAL:HG13	1.65	0.78
1:F:111:ASN:ND2	1:F:115:ASN:OD1	2.17	0.77
1:D:173:HIS:ND1	1:D:173:HIS:O	2.17	0.77
1:H:128:ASN:OD1	1:H:359:LYS:NZ	2.13	0.77
2:A:637:THR:HG22	2:A:639:LEU:H	1.50	0.77
2:A:789:LYS:O	2:A:792:SER:OG	2.03	0.76
2:B:789:LYS:O	2:B:792:SER:OG	2.01	0.76
1:F:173:HIS:ND1	1:F:173:HIS:O	2.19	0.75
2:C:758:LYS:HB2	2:C:898:VAL:HG13	1.68	0.75
1:H:173:HIS:O	1:H:173:HIS:ND1	2.20	0.74
2:E:765:GLN:HG2	2:E:823:LEU:HD11	1.69	0.74
1:G:173:HIS:O	1:G:173:HIS:ND1	2.19	0.74
2:B:758:LYS:HB2	2:B:898:VAL:HG13	1.70	0.74
1:G:164:PRO:HG2	1:G:174:ALA:HB1	1.69	0.73
1:D:164:PRO:HG2	1:D:174:ALA:HB1	1.69	0.73
1:F:106:THR:HB	1:F:137:GLN:HG2	1.71	0.73
2:C:637:THR:HG22	2:C:639:LEU:H	1.52	0.73
2:E:637:THR:HG22	2:E:639:LEU:H	1.54	0.73
2:E:807:THR:HG23	2:E:810:HIS:H	1.52	0.73
2:B:765:GLN:HG2	2:B:823:LEU:HD11	1.71	0.72
2:C:807:THR:HG23	2:C:810:HIS:H	1.53	0.72
1:G:106:THR:HB	1:G:137:GLN:HG2	1.71	0.72
1:D:106:THR:HB	1:D:137:GLN:HG2	1.71	0.72
2:A:765:GLN:HG2	2:A:823:LEU:HD11	1.71	0.72
2:B:637:THR:HG22	2:B:639:LEU:H	1.55	0.71
2:B:757:VAL:HA	2:B:830:LEU:HD23	1.72	0.71
1:F:20:GLY:HA2	1:F:94:LEU:HD21	1.70	0.71
2:E:598:LEU:HD12	2:E:599:GLU:H	1.55	0.71
1:H:164:PRO:HG2	1:H:174:ALA:HB1	1.72	0.71
2:C:598:LEU:HD12	2:C:599:GLU:H	1.55	0.71
1:H:106:THR:HB	1:H:137:GLN:HG2	1.71	0.71
2:A:807:THR:HG23	2:A:810:HIS:H	1.54	0.71
2:C:746:GLN:HE22	1:F:323:SER:HB3	1.55	0.71
1:G:20:GLY:HA2	1:G:94:LEU:HD21	1.73	0.71
2:B:598:LEU:HD12	2:B:599:GLU:H	1.57	0.70
1:H:20:GLY:HA2	1:H:94:LEU:HD21	1.73	0.70
1:F:16:LEU:HD12	1:F:32:PRO:HA	1.73	0.70
2:C:757:VAL:HA	2:C:830:LEU:HD23	1.73	0.70
1:H:111:ASN:ND2	1:H:115:ASN:OD1	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:SER:HB3	2:A:746:GLN:HE22	1.56	0.70
2:B:565:ILE:HD13	2:B:566:LYS:H	1.55	0.70
1:G:25:ASP:OD2	1:G:28:ARG:NH2	2.24	0.69
1:G:25:ASP:N	3:G:401:ACT:OXT	2.24	0.69
2:C:643:ARG:NH2	2:C:690:GLU:OE2	2.24	0.69
1:G:16:LEU:HD12	1:G:32:PRO:HA	1.74	0.69
1:G:260:THR:HG23	1:G:266:PHE:HB2	1.73	0.69
1:H:16:LEU:HD12	1:H:32:PRO:HA	1.74	0.69
1:D:20:GLY:HA2	1:D:94:LEU:HD21	1.73	0.69
2:B:643:ARG:NH2	2:B:690:GLU:OE2	2.26	0.69
2:A:598:LEU:HD12	2:A:599:GLU:H	1.55	0.69
2:E:746:GLN:HE22	1:G:323:SER:HB3	1.57	0.69
2:E:858:ILE:HG22	2:E:874:LEU:HD12	1.75	0.69
2:A:645:LYS:NZ	2:A:646:ASN:OD1	2.25	0.69
2:A:757:VAL:HA	2:A:830:LEU:HD23	1.74	0.69
1:F:260:THR:HG23	1:F:266:PHE:HB2	1.75	0.68
2:E:757:VAL:HA	2:E:830:LEU:HD23	1.73	0.68
1:F:164:PRO:HG2	1:F:174:ALA:HB1	1.75	0.68
1:D:278:THR:O	1:D:282:ILE:HD12	1.93	0.68
2:E:643:ARG:NH2	2:E:690:GLU:OE2	2.27	0.68
2:A:669:ASP:HB3	2:A:673:LEU:HB2	1.76	0.67
1:D:128:ASN:OD1	1:D:359:LYS:NZ	2.18	0.67
1:G:111:ASN:ND2	1:G:115:ASN:OD1	2.25	0.67
2:A:643:ARG:NH2	2:A:690:GLU:OE2	2.28	0.67
2:C:765:GLN:HG2	2:C:823:LEU:HD11	1.77	0.67
2:B:605:ARG:HG2	2:B:609:LEU:HD12	1.77	0.67
2:B:840:SER:N	1:H:323:SER:OG	2.20	0.67
1:H:25:ASP:OD2	1:H:28:ARG:NH2	2.27	0.67
1:H:217:CYS:HA	1:H:254:ARG:HG3	1.75	0.67
1:G:128:ASN:OD1	1:G:359:LYS:NZ	2.17	0.67
1:D:136:ILE:H	1:D:136:ILE:HD12	1.60	0.67
1:H:107:GLU:O	1:H:137:GLN:HG3	1.95	0.66
1:G:157:ASP:HB2	4:G:402:ATP:H5'1	1.77	0.66
2:A:605:ARG:HG2	2:A:609:LEU:HD12	1.77	0.66
1:G:217:CYS:HA	1:G:254:ARG:HG3	1.77	0.66
2:A:858:ILE:HG22	2:A:874:LEU:HD12	1.77	0.66
2:E:823:LEU:O	2:E:826:PHE:HB3	1.97	0.65
1:G:136:ILE:HD12	1:G:136:ILE:H	1.61	0.65
2:B:823:LEU:O	2:B:826:PHE:HB3	1.96	0.65
1:D:260:THR:HG23	1:D:266:PHE:HB2	1.79	0.64
1:D:111:ASN:ND2	1:D:115:ASN:OD1	2.24	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LEU:HD12	1:D:32:PRO:HA	1.78	0.64
2:C:823:LEU:O	2:C:826:PHE:HB3	1.96	0.64
1:F:136:ILE:HD12	1:F:136:ILE:H	1.63	0.64
1:F:217:CYS:HA	1:F:254:ARG:HG3	1.78	0.64
1:F:25:ASP:OD2	1:F:28:ARG:NH2	2.30	0.64
1:H:136:ILE:HD12	1:H:136:ILE:H	1.62	0.64
2:C:858:ILE:HG22	2:C:874:LEU:HD12	1.79	0.64
2:E:605:ARG:HG2	2:E:609:LEU:HD12	1.79	0.64
2:C:866:ASP:N	2:C:867:ASN:OD1	2.31	0.64
1:D:25:ASP:OD2	1:D:28:ARG:NH2	2.31	0.64
2:C:669:ASP:HB3	2:C:673:LEU:HB2	1.79	0.64
2:A:823:LEU:O	2:A:826:PHE:HB3	1.98	0.64
1:H:260:THR:HG23	1:H:266:PHE:HB2	1.80	0.64
1:D:157:ASP:HB2	4:D:402:ATP:H5'1	1.79	0.63
1:H:96:VAL:HB	1:H:101:HIS:CE1	2.33	0.63
2:C:762:LYS:HB3	2:C:826:PHE:HB2	1.78	0.63
1:D:217:CYS:HA	1:D:254:ARG:HG3	1.79	0.63
2:A:654:ALA:HB2	2:A:677:PHE:CE1	2.34	0.63
2:A:762:LYS:HB3	2:A:826:PHE:HB2	1.80	0.63
1:D:25:ASP:N	3:D:401:ACT:OXT	2.32	0.63
2:E:654:ALA:HB2	2:E:677:PHE:CE1	2.33	0.63
2:E:669:ASP:HB3	2:E:673:LEU:HB2	1.81	0.63
1:D:107:GLU:O	1:D:137:GLN:HG3	1.99	0.63
2:B:866:ASP:N	2:B:867:ASN:OD1	2.32	0.63
2:A:866:ASP:N	2:A:867:ASN:OD1	2.31	0.63
2:B:858:ILE:HG22	2:B:874:LEU:HD12	1.80	0.62
2:B:638:LEU:N	2:B:711:ASP:OD2	2.18	0.62
2:B:762:LYS:HB3	2:B:826:PHE:HB2	1.81	0.62
2:C:654:ALA:HB2	2:C:677:PHE:CE1	2.34	0.62
2:C:789:LYS:HG3	2:B:579:LEU:HD21	1.80	0.62
1:H:18:LYS:HA	1:H:30:VAL:HG22	1.82	0.62
2:C:913:VAL:O	2:C:916:PRO:HD2	2.00	0.61
2:A:576:TRP:HB2	2:E:792:SER:HB3	1.82	0.61
2:A:782:ARG:NH1	2:E:573:VAL:HG23	2.15	0.61
1:F:138:ALA:O	1:F:152:VAL:HG21	1.99	0.61
2:B:654:ALA:HB2	2:B:677:PHE:CE1	2.35	0.61
2:E:771:LEU:O	2:E:775:ASN:HB2	2.01	0.61
1:D:367:PRO:HD3	2:A:573:VAL:HG11	1.83	0.61
2:A:672:THR:O	2:A:672:THR:OG1	2.15	0.61
2:C:779:SER:HB3	2:B:565:ILE:H	1.64	0.61
1:F:186:THR:O	1:F:190:MET:HG2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:LYS:HA	1:G:30:VAL:HG22	1.82	0.61
2:C:743:LEU:HD22	2:C:844:VAL:HG13	1.81	0.61
1:D:138:ALA:O	1:D:152:VAL:HG21	2.01	0.61
2:E:869:VAL:HA	2:E:872:ASN:HB3	1.83	0.61
2:B:645:LYS:NZ	2:B:646:ASN:OD1	2.34	0.60
2:A:913:VAL:O	2:A:916:PRO:HD2	2.01	0.60
2:B:669:ASP:HB3	2:B:673:LEU:HB2	1.83	0.60
2:E:866:ASP:N	2:E:867:ASN:OD1	2.35	0.60
2:A:573:VAL:HG23	2:E:782:ARG:NH1	2.16	0.60
2:E:743:LEU:HD22	2:E:844:VAL:HG13	1.83	0.60
1:D:137:GLN:NE2	4:D:402:ATP:O3G	2.35	0.60
1:G:272:ALA:HB1	1:G:276:GLU:HB2	1.82	0.60
1:G:278:THR:O	1:G:282:ILE:HD12	2.02	0.60
1:G:96:VAL:HB	1:G:101:HIS:CE1	2.37	0.60
2:C:579:LEU:HD21	2:B:789:LYS:HG3	1.84	0.60
2:E:762:LYS:HB3	2:E:826:PHE:HB2	1.83	0.60
1:G:280:ASN:HA	1:G:283:MET:HB2	1.84	0.60
2:C:605:ARG:HG2	2:C:609:LEU:HD12	1.83	0.59
2:C:638:LEU:N	2:C:711:ASP:OD2	2.21	0.59
1:G:107:GLU:O	1:G:137:GLN:HG3	2.01	0.59
2:A:578:ALA:HB1	2:E:785:VAL:HG21	1.83	0.59
1:F:18:LYS:HA	1:F:30:VAL:HG22	1.85	0.59
1:H:27:PRO:HD3	1:H:340:TRP:CE3	2.38	0.59
2:A:743:LEU:HD22	2:A:844:VAL:HG13	1.83	0.59
2:A:722:ARG:HA	2:A:722:ARG:NH1	2.18	0.59
2:A:875:SER:OG	2:A:876:THR:N	2.36	0.59
2:B:869:VAL:HA	2:B:872:ASN:HB3	1.84	0.58
2:C:869:VAL:HA	2:C:872:ASN:HB3	1.84	0.58
1:G:186:THR:O	1:G:190:MET:HG2	2.03	0.58
1:H:186:THR:O	1:H:190:MET:HG2	2.03	0.58
2:A:771:LEU:O	2:A:775:ASN:HB2	2.04	0.58
1:G:27:PRO:HD3	1:G:340:TRP:CE3	2.39	0.58
2:B:743:LEU:HD22	2:B:844:VAL:HG13	1.85	0.58
2:B:576:TRP:HD1	2:B:576:TRP:O	1.86	0.58
2:C:771:LEU:O	2:C:775:ASN:HB2	2.03	0.58
1:D:186:THR:O	1:D:190:MET:HG2	2.03	0.58
2:C:778:ASN:ND2	3:B:1001:ACT:O	2.37	0.57
1:H:222:ASP:HB3	1:H:225:ASN:HB2	1.86	0.57
2:B:913:VAL:O	2:B:916:PRO:HD2	2.03	0.57
1:F:96:VAL:HB	1:F:101:HIS:CE1	2.40	0.57
1:D:222:ASP:HB3	1:D:225:ASN:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:869:VAL:HA	2:A:872:ASN:HB3	1.85	0.57
1:F:222:ASP:HB3	1:F:225:ASN:HB2	1.87	0.57
1:D:18:LYS:HA	1:D:30:VAL:HG22	1.86	0.57
1:D:96:VAL:HB	1:D:101:HIS:CE1	2.39	0.57
2:E:576:TRP:HD1	2:E:576:TRP:O	1.86	0.57
2:B:664:ALA:HA	2:B:667:THR:HG22	1.86	0.57
1:F:9:VAL:HG12	1:F:340:TRP:NE1	2.19	0.57
1:G:138:ALA:O	1:G:152:VAL:HG21	2.05	0.57
1:D:9:VAL:HG22	1:D:104:LEU:HB3	1.86	0.57
2:B:570:ARG:O	2:B:570:ARG:HG3	2.04	0.57
2:C:576:TRP:O	2:C:576:TRP:HD1	1.87	0.57
2:C:570:ARG:HG3	2:C:570:ARG:O	2.04	0.57
1:G:222:ASP:HB3	1:G:225:ASN:HB2	1.86	0.57
1:F:333:PRO:HG2	1:F:334:GLU:HG3	1.87	0.57
1:G:9:VAL:HG22	1:G:104:LEU:HB3	1.87	0.57
2:C:565:ILE:HD13	2:C:566:LYS:H	1.69	0.56
2:C:568:LYS:HB3	2:C:569:PHE:HD1	1.70	0.56
2:A:576:TRP:O	2:A:576:TRP:HD1	1.88	0.56
1:G:151:ILE:HD12	1:G:164:PRO:HG3	1.88	0.56
2:A:578:ALA:HB1	2:E:785:VAL:HG11	1.87	0.56
1:F:107:GLU:O	1:F:137:GLN:HG3	2.05	0.56
2:C:672:THR:OG1	2:C:672:THR:O	2.11	0.56
2:C:807:THR:OG1	2:C:808:LEU:N	2.38	0.56
2:B:740:LEU:HB2	2:B:884:LEU:HD13	1.87	0.56
2:A:568:LYS:HB3	2:A:569:PHE:HD1	1.70	0.56
2:E:638:LEU:N	2:E:711:ASP:OD2	2.23	0.56
2:C:875:SER:OG	2:C:876:THR:N	2.37	0.56
2:E:649:ILE:HD13	1:G:143:TYR:CE1	2.41	0.56
1:H:218:TYR:CZ	1:H:255:PHE:HB3	2.42	0.55
2:A:570:ARG:HG3	2:A:570:ARG:O	2.07	0.55
1:D:280:ASN:HA	1:D:283:MET:HB2	1.88	0.55
2:E:573:VAL:HG11	1:G:367:PRO:HD3	1.89	0.55
1:D:272:ALA:HB1	1:D:276:GLU:HB2	1.86	0.55
1:H:147:ARG:NH1	1:H:330:ILE:HG12	2.12	0.55
2:B:565:ILE:CD1	2:B:566:LYS:H	2.19	0.55
2:B:771:LEU:O	2:B:775:ASN:HB2	2.06	0.55
1:H:272:ALA:HB1	1:H:276:GLU:HB2	1.87	0.55
1:F:71:ILE:HG23	1:F:76:ILE:HG12	1.88	0.55
2:E:570:ARG:O	2:E:570:ARG:HG3	2.07	0.55
1:H:138:ALA:O	1:H:152:VAL:HG21	2.05	0.55
1:F:278:THR:O	1:F:282:ILE:HD12	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ASN:HA	1:F:283:MET:HB2	1.88	0.55
2:C:664:ALA:HA	2:C:667:THR:HG22	1.88	0.55
2:E:568:LYS:HB3	2:E:569:PHE:HD1	1.71	0.55
1:D:14:SER:OG	4:D:402:ATP:O2B	2.25	0.55
2:A:866:ASP:HB3	2:A:867:ASN:HA	1.89	0.55
1:D:71:ILE:HG23	1:D:76:ILE:HG12	1.89	0.54
2:E:913:VAL:O	2:E:916:PRO:HD2	2.07	0.54
2:C:905:SER:O	2:C:909:THR:HG23	2.08	0.54
1:H:71:ILE:HG23	1:H:76:ILE:HG12	1.88	0.54
2:E:645:LYS:NZ	2:E:646:ASN:OD1	2.41	0.54
1:F:14:SER:OG	4:F:403:ATP:O2B	2.23	0.54
1:D:151:ILE:HD12	1:D:164:PRO:HG3	1.89	0.54
1:H:278:THR:O	1:H:282:ILE:HD12	2.08	0.54
1:F:35:VAL:HG21	1:F:81:ASP:HB3	1.88	0.54
1:F:287:ILE:HG23	1:F:290:ARG:NH1	2.22	0.54
1:H:280:ASN:HA	1:H:283:MET:HB2	1.89	0.54
1:G:274:ILE:HG21	1:G:313:MET:HE1	1.89	0.54
2:A:638:LEU:N	2:A:711:ASP:OD2	2.24	0.54
2:A:792:SER:HB3	2:E:576:TRP:HB2	1.91	0.53
1:H:9:VAL:HG12	1:H:340:TRP:NE1	2.23	0.53
1:H:151:ILE:HD12	1:H:164:PRO:HG3	1.91	0.53
1:H:27:PRO:HD3	1:H:340:TRP:CD2	2.43	0.53
1:D:143:TYR:CE1	2:A:649:ILE:HD13	2.43	0.53
1:G:71:ILE:HG23	1:G:76:ILE:HG12	1.89	0.53
1:G:260:THR:HG21	1:G:267:ILE:HG23	1.90	0.53
2:E:672:THR:OG1	2:E:672:THR:O	2.18	0.53
1:G:287:ILE:HA	1:G:290:ARG:HD3	1.91	0.53
2:B:568:LYS:HB3	2:B:569:PHE:HD1	1.74	0.53
2:A:905:SER:O	2:A:909:THR:HG23	2.08	0.53
2:C:813:ALA:HB3	2:C:932:ASN:ND2	2.24	0.53
1:D:287:ILE:HA	1:D:290:ARG:HD3	1.90	0.53
1:F:151:ILE:HD12	1:F:164:PRO:HG3	1.91	0.53
1:G:178:LEU:HG	1:G:180:LEU:H	1.74	0.53
2:A:827:TRP:CD1	2:A:828:GLN:HG3	2.43	0.53
1:H:17:VAL:O	1:H:30:VAL:HA	2.09	0.53
1:D:218:TYR:CZ	1:D:255:PHE:HB3	2.43	0.53
2:C:785:VAL:HG21	2:B:578:ALA:HB1	1.91	0.53
1:F:287:ILE:HA	1:F:290:ARG:HD3	1.91	0.53
1:G:196:ARG:HH21	1:G:251:GLY:H	1.57	0.53
2:B:905:SER:O	2:B:909:THR:HG23	2.08	0.53
2:C:827:TRP:CZ3	2:C:926:LYS:HG2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:840:SER:N	1:G:323:SER:OG	2.33	0.52
2:C:866:ASP:HB3	2:C:867:ASN:HA	1.90	0.52
2:E:664:ALA:HA	2:E:667:THR:HG22	1.91	0.52
2:B:713:PHE:O	2:B:717:PHE:HB2	2.08	0.52
2:C:573:VAL:HG11	1:F:367:PRO:HD3	1.91	0.52
1:G:264:PRO:HG2	1:G:271:SER:O	2.09	0.52
2:B:813:ALA:HB3	2:B:932:ASN:ND2	2.25	0.52
1:D:287:ILE:HG23	1:D:290:ARG:NH1	2.25	0.52
1:F:272:ALA:HB1	1:F:276:GLU:HB2	1.90	0.52
2:E:859:ARG:HB3	2:E:874:LEU:HD11	1.92	0.52
1:G:264:PRO:HG3	1:G:273:GLY:HA2	1.90	0.52
1:D:116:ARG:HG3	1:D:134:VAL:HG11	1.90	0.52
2:B:722:ARG:NH1	2:B:725:GLN:OE1	2.36	0.52
2:B:807:THR:OG1	2:B:808:LEU:N	2.43	0.52
2:B:866:ASP:HB3	2:B:867:ASN:HA	1.91	0.52
2:E:866:ASP:HB3	2:E:867:ASN:HA	1.91	0.52
1:G:333:PRO:HG2	1:G:334:GLU:HG3	1.92	0.52
1:G:218:TYR:CZ	1:G:255:PHE:HB3	2.45	0.52
1:F:260:THR:HG21	1:F:267:ILE:HG23	1.91	0.52
2:B:692:LYS:HA	2:B:695:ARG:HG2	1.91	0.52
2:C:565:ILE:H	2:B:779:SER:HB3	1.75	0.51
1:G:287:ILE:HG23	1:G:290:ARG:NH1	2.25	0.51
2:E:827:TRP:CD1	2:E:828:GLN:HG3	2.45	0.51
1:F:292:ASP:OD1	1:F:292:ASP:N	2.43	0.51
1:G:116:ARG:HG3	1:G:134:VAL:HG11	1.92	0.51
2:C:859:ARG:HB3	2:C:874:LEU:HD11	1.92	0.51
1:F:27:PRO:HD3	1:F:340:TRP:CE3	2.46	0.51
2:C:827:TRP:CD1	2:C:828:GLN:HG3	2.45	0.51
1:F:218:TYR:CZ	1:F:255:PHE:HB3	2.45	0.51
1:H:9:VAL:HG22	1:H:104:LEU:HB3	1.92	0.51
1:D:264:PRO:HG2	1:D:271:SER:O	2.11	0.51
2:E:905:SER:O	2:E:909:THR:HG23	2.10	0.51
1:H:287:ILE:HG23	1:H:290:ARG:NH1	2.25	0.51
2:A:664:ALA:HA	2:A:667:THR:HG22	1.91	0.51
2:E:737:GLN:O	2:E:741:GLN:HG2	2.11	0.51
2:E:899:VAL:HG22	2:E:914:PHE:CD1	2.45	0.51
2:B:722:ARG:HA	2:B:722:ARG:NH1	2.25	0.51
2:C:740:LEU:HB2	2:C:884:LEU:HD13	1.92	0.51
1:F:9:VAL:HG12	1:F:340:TRP:CD1	2.46	0.51
2:B:827:TRP:CD1	2:B:828:GLN:HG3	2.45	0.51
2:C:761:GLN:CD	2:C:761:GLN:H	2.14	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:HIS:HB3	1:H:177:ARG:HH22	1.75	0.51
2:B:746:GLN:NE2	1:H:323:SER:HB3	2.19	0.51
1:F:264:PRO:HG2	1:F:271:SER:O	2.11	0.51
2:B:859:ARG:HB3	2:B:874:LEU:HD11	1.93	0.50
1:D:9:VAL:HG12	1:D:340:TRP:NE1	2.26	0.50
2:B:875:SER:OG	2:B:876:THR:N	2.43	0.50
2:A:750:ILE:O	2:A:754:SER:HB3	2.11	0.50
1:H:313:MET:O	1:H:317:ILE:HG12	2.11	0.50
1:D:125:GLU:OE1	3:E:1001:ACT:H2	2.10	0.50
1:D:17:VAL:O	1:D:30:VAL:HA	2.12	0.50
2:C:722:ARG:HA	2:C:722:ARG:NH1	2.26	0.50
1:D:274:ILE:HG21	1:D:313:MET:HE1	1.93	0.50
1:H:9:VAL:HG12	1:H:340:TRP:CD1	2.46	0.50
1:H:157:ASP:OD2	1:H:183:ARG:NH1	2.44	0.50
2:A:859:ARG:HB3	2:A:874:LEU:HD11	1.94	0.50
2:A:775:ASN:ND2	2:A:785:VAL:O	2.36	0.50
1:G:9:VAL:HG12	1:G:340:TRP:NE1	2.27	0.50
2:B:825:ASN:O	2:B:827:TRP:N	2.44	0.50
2:E:813:ALA:HB3	2:E:932:ASN:ND2	2.27	0.50
1:G:8:LEU:HD11	1:G:94:LEU:CD1	2.42	0.50
2:E:827:TRP:CD1	2:E:828:GLN:N	2.80	0.50
1:H:287:ILE:HA	1:H:290:ARG:HD3	1.92	0.50
1:D:315:LYS:HG3	1:D:316:GLU:N	2.25	0.50
2:B:573:VAL:HG12	1:H:125:GLU:OE2	2.12	0.50
2:E:716:LEU:O	2:E:719:LYS:HB2	2.12	0.50
2:A:825:ASN:O	2:A:827:TRP:N	2.43	0.49
1:D:264:PRO:HG3	1:D:273:GLY:HA2	1.94	0.49
1:H:315:LYS:HG3	1:H:316:GLU:N	2.27	0.49
2:E:750:ILE:O	2:E:754:SER:HB3	2.12	0.49
1:G:35:VAL:HG21	1:G:81:ASP:HB3	1.92	0.49
1:F:291:LYS:HZ2	1:F:325:MET:HA	1.76	0.49
1:H:35:VAL:HG21	1:H:81:ASP:HB3	1.94	0.49
1:H:89:THR:O	1:H:94:LEU:HB2	2.13	0.49
1:H:125:GLU:OE2	1:H:362:TYR:OH	2.31	0.49
1:H:178:LEU:HG	1:H:180:LEU:H	1.77	0.49
1:G:315:LYS:HG3	1:G:316:GLU:N	2.27	0.49
1:D:27:PRO:HD3	1:D:340:TRP:CE3	2.47	0.49
1:H:333:PRO:HG2	1:H:334:GLU:HG3	1.95	0.49
2:E:875:SER:OG	2:E:876:THR:N	2.46	0.49
2:B:738:ASP:O	2:B:741:GLN:HB2	2.12	0.49
2:A:761:GLN:CD	2:A:761:GLN:H	2.15	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:722:ARG:NH1	2:C:725:GLN:OE1	2.38	0.49
1:H:350:SER:O	1:H:353:GLN:HG2	2.13	0.49
1:H:264:PRO:HG2	1:H:271:SER:O	2.11	0.49
1:G:17:VAL:O	1:G:30:VAL:HA	2.12	0.49
1:G:196:ARG:HG3	1:G:253:GLU:HG3	1.94	0.49
2:B:716:LEU:O	2:B:719:LYS:HB2	2.13	0.49
1:F:313:MET:O	1:F:317:ILE:HG12	2.13	0.49
2:B:807:THR:HG22	2:B:810:HIS:ND1	2.28	0.49
1:G:27:PRO:HD3	1:G:340:TRP:CD2	2.47	0.49
2:C:576:TRP:HB2	2:B:792:SER:HB3	1.93	0.49
1:G:25:ASP:HB3	3:G:401:ACT:O	2.12	0.49
1:D:238:LYS:HB2	1:D:254:ARG:NH1	2.28	0.49
3:C:1001:ACT:OXT	2:B:778:ASN:ND2	2.45	0.49
2:A:716:LEU:O	2:A:719:LYS:HB2	2.13	0.49
1:G:147:ARG:NH1	1:G:330:ILE:HG12	2.17	0.49
1:G:173:HIS:CG	1:G:173:HIS:O	2.65	0.49
2:C:913:VAL:HG23	2:C:914:PHE:N	2.28	0.49
1:G:276:GLU:O	1:G:279:TYR:N	2.45	0.49
1:G:10:CYS:O	1:G:105:LEU:HA	2.13	0.49
1:H:264:PRO:HG3	1:H:273:GLY:HA2	1.93	0.49
2:E:790:LEU:HG	2:E:917:VAL:HG11	1.94	0.49
2:C:833:VAL:HG23	2:C:915:PHE:HB3	1.95	0.49
2:B:833:VAL:HG23	2:B:915:PHE:HB3	1.95	0.49
2:A:692:LYS:HA	2:A:695:ARG:HG2	1.93	0.49
2:A:813:ALA:HB3	2:A:932:ASN:ND2	2.27	0.49
2:E:808:LEU:O	2:E:812:ILE:HG13	2.13	0.48
2:B:647:LEU:HD22	2:B:651:LEU:HG	1.95	0.48
1:F:17:VAL:HG23	1:F:33:SER:HB3	1.95	0.48
2:C:840:SER:N	1:F:323:SER:OG	2.34	0.48
1:F:173:HIS:CG	1:F:173:HIS:O	2.64	0.48
1:H:25:ASP:N	3:H:401:ACT:OXT	2.46	0.48
2:A:722:ARG:HA	2:A:722:ARG:CZ	2.42	0.48
2:C:775:ASN:ND2	2:C:785:VAL:O	2.35	0.48
2:C:578:ALA:HB1	2:B:785:VAL:HG21	1.94	0.48
2:C:825:ASN:O	2:C:827:TRP:N	2.40	0.48
1:F:330:ILE:HG22	1:F:332:PRO:HD3	1.95	0.48
1:G:89:THR:O	1:G:94:LEU:HB2	2.13	0.48
1:D:73:HIS:HB3	1:D:177:ARG:HH22	1.79	0.48
2:E:795:LEU:H	2:E:795:LEU:HD23	1.78	0.48
2:A:808:LEU:O	2:A:812:ILE:HG13	2.14	0.48
1:D:178:LEU:HG	1:D:180:LEU:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:ASP:OD2	1:G:183:ARG:NH1	2.47	0.48
2:A:722:ARG:NH1	2:A:725:GLN:OE1	2.39	0.48
1:F:276:GLU:O	1:F:279:TYR:N	2.47	0.48
2:C:649:ILE:HD13	1:F:143:TYR:CE1	2.49	0.48
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.95	0.48
1:F:8:LEU:HD11	1:F:94:LEU:CD1	2.43	0.48
1:F:262:PHE:HD1	1:F:275:HIS:ND1	2.12	0.48
1:D:196:ARG:HG3	1:D:253:GLU:HG3	1.95	0.48
2:C:877:ASN:O	2:C:880:LYS:N	2.45	0.48
2:B:575:ASN:HA	3:B:1001:ACT:H2	1.94	0.48
2:C:746:GLN:NE2	1:F:323:SER:HB3	2.27	0.48
2:C:716:LEU:O	2:C:719:LYS:HB2	2.14	0.48
2:C:713:PHE:O	2:C:717:PHE:HB2	2.14	0.48
2:A:574:PHE:CE2	2:A:576:TRP:HB3	2.49	0.48
2:A:807:THR:OG1	2:A:808:LEU:N	2.45	0.48
1:F:76:ILE:HD13	1:F:82:MET:HG2	1.96	0.48
2:A:740:LEU:HB2	2:A:884:LEU:HD13	1.95	0.48
1:H:10:CYS:O	1:H:105:LEU:HA	2.14	0.48
1:F:73:HIS:HB3	1:F:177:ARG:HH22	1.78	0.48
1:F:118:LYS:O	1:F:122:ILE:HG13	2.13	0.48
1:H:292:ASP:OD1	1:H:292:ASP:N	2.47	0.48
1:H:173:HIS:O	1:H:173:HIS:CG	2.65	0.47
2:E:779:SER:O	2:E:780:SER:OG	2.26	0.47
1:D:288:ASP:OD1	1:D:288:ASP:N	2.47	0.47
1:G:292:ASP:N	1:G:292:ASP:OD1	2.47	0.47
1:D:313:MET:O	1:D:317:ILE:HG12	2.14	0.47
2:A:827:TRP:NE1	2:A:828:GLN:HG3	2.29	0.47
2:A:647:LEU:HD22	2:A:651:LEU:HG	1.96	0.47
2:B:795:LEU:H	2:B:795:LEU:HD23	1.79	0.47
2:C:899:VAL:HG22	2:C:914:PHE:CD1	2.49	0.47
2:E:647:LEU:HD22	2:E:651:LEU:HG	1.96	0.47
2:A:795:LEU:H	2:A:795:LEU:HD23	1.80	0.47
2:E:713:PHE:O	2:E:717:PHE:HB2	2.14	0.47
2:C:808:LEU:O	2:C:812:ILE:HG13	2.15	0.47
1:D:323:SER:HB3	2:A:746:GLN:NE2	2.27	0.47
2:B:913:VAL:HG23	2:B:914:PHE:N	2.30	0.47
1:H:262:PHE:HD1	1:H:275:HIS:ND1	2.12	0.47
1:H:242:LEU:HD22	1:H:246:GLN:HG3	1.96	0.47
1:H:8:LEU:HD11	1:H:94:LEU:CD1	2.45	0.47
2:B:573:VAL:HG11	1:H:367:PRO:HD3	1.97	0.47
2:A:894:ALA:O	2:A:897:ALA:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:738:ASP:O	2:E:741:GLN:HB2	2.14	0.47
1:G:125:GLU:OE2	1:G:362:TYR:OH	2.33	0.47
1:D:35:VAL:HG21	1:D:81:ASP:HB3	1.96	0.47
1:D:173:HIS:O	1:D:173:HIS:CG	2.62	0.47
2:C:565:ILE:CD1	2:C:566:LYS:H	2.27	0.47
2:B:750:ILE:O	2:B:754:SER:HB3	2.15	0.47
1:D:292:ASP:OD1	1:D:292:ASP:N	2.47	0.47
3:C:1002:ACT:OXT	1:H:121:GLN:NE2	2.47	0.47
1:G:17:VAL:HG23	1:G:33:SER:HB3	1.97	0.47
1:G:73:HIS:HB3	1:G:177:ARG:HH22	1.78	0.47
1:D:295:ALA:O	1:D:328:LYS:HB3	2.15	0.47
1:H:238:LYS:HB2	1:H:254:ARG:NH1	2.29	0.47
1:H:260:THR:HG21	1:H:267:ILE:HG23	1.97	0.47
1:F:9:VAL:HG22	1:F:104:LEU:HB3	1.97	0.47
1:G:361:GLU:H	1:G:361:GLU:HG2	1.49	0.47
2:E:807:THR:OG1	2:E:808:LEU:N	2.48	0.47
1:G:9:VAL:HG12	1:G:340:TRP:CD1	2.50	0.47
2:B:899:VAL:HG22	2:B:914:PHE:CD1	2.49	0.47
1:F:219:VAL:HG22	1:F:258:PRO:HB2	1.96	0.47
2:C:750:ILE:O	2:C:754:SER:HB3	2.14	0.47
1:F:17:VAL:O	1:F:30:VAL:HA	2.15	0.46
2:A:827:TRP:CD1	2:A:828:GLN:N	2.83	0.46
2:C:827:TRP:CD1	2:C:828:GLN:N	2.83	0.46
2:E:656:ARG:HB3	2:E:661:ILE:HG13	1.97	0.46
2:A:816:VAL:HG11	2:A:925:TYR:OH	2.15	0.46
1:F:125:GLU:OE2	1:F:362:TYR:OH	2.33	0.46
2:E:796:LEU:HA	2:E:796:LEU:HD23	1.61	0.46
2:B:808:LEU:O	2:B:812:ILE:HG13	2.15	0.46
2:A:578:ALA:CB	2:E:785:VAL:HG11	2.45	0.46
1:G:242:LEU:HD22	1:G:246:GLN:HG3	1.97	0.46
2:B:609:LEU:C	2:B:610:PHE:HD1	2.19	0.46
1:H:276:GLU:O	1:H:279:TYR:N	2.49	0.46
1:H:73:HIS:HB3	1:H:177:ARG:NH2	2.30	0.46
1:F:140:LEU:O	1:F:342:GLY:HA3	2.16	0.46
1:D:89:THR:O	1:D:94:LEU:HB2	2.15	0.46
1:G:112:PRO:HD2	1:G:115:ASN:HB2	1.98	0.46
2:E:827:TRP:NE1	2:E:828:GLN:HG3	2.31	0.46
1:G:316:GLU:O	1:G:320:LEU:HD13	2.16	0.46
1:G:140:LEU:O	1:G:342:GLY:HA3	2.16	0.46
1:F:264:PRO:HG3	1:F:273:GLY:HA2	1.98	0.46
1:D:147:ARG:NH1	1:D:330:ILE:HG12	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:306:TYR:CE1	4:H:402:ATP:H2	2.32	0.46
2:E:775:ASN:ND2	2:E:785:VAL:O	2.36	0.46
2:C:795:LEU:H	2:C:795:LEU:HD23	1.81	0.46
1:D:262:PHE:HD1	1:D:275:HIS:ND1	2.14	0.46
2:B:827:TRP:NE1	2:B:828:GLN:HG3	2.31	0.46
2:B:877:ASN:O	2:B:880:LYS:N	2.48	0.46
2:A:713:PHE:O	2:A:717:PHE:HB2	2.14	0.46
2:E:825:ASN:O	2:E:827:TRP:N	2.42	0.46
1:D:330:ILE:HG22	1:D:332:PRO:HD3	1.97	0.46
1:G:262:PHE:HD1	1:G:275:HIS:ND1	2.14	0.46
1:H:275:HIS:CD2	1:H:276:GLU:HG3	2.51	0.46
1:D:76:ILE:HD13	1:D:82:MET:HG2	1.97	0.46
1:G:160:THR:HB	1:G:178:LEU:HB3	1.98	0.46
1:H:261:LEU:HB3	1:H:274:ILE:CD1	2.37	0.46
1:H:158:GLY:HA3	1:H:183:ARG:NH2	2.31	0.46
2:C:646:ASN:HB3	1:F:148:THR:HG21	1.97	0.46
1:F:242:LEU:HD22	1:F:246:GLN:HG3	1.96	0.46
1:D:9:VAL:HG12	1:D:340:TRP:CD1	2.51	0.45
2:B:775:ASN:ND2	2:B:785:VAL:O	2.36	0.45
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.98	0.45
1:D:291:LYS:HZ2	1:D:325:MET:HA	1.81	0.45
1:F:10:CYS:O	1:F:105:LEU:HA	2.16	0.45
1:F:111:ASN:HA	1:F:112:PRO:HD3	1.67	0.45
1:H:219:VAL:HG22	1:H:258:PRO:HB2	1.98	0.45
1:D:140:LEU:O	1:D:342:GLY:HA3	2.16	0.45
1:H:330:ILE:HG22	1:H:332:PRO:HD3	1.97	0.45
1:G:330:ILE:HG22	1:G:332:PRO:HD3	1.98	0.45
1:D:306:TYR:CE1	4:D:402:ATP:H2	2.34	0.45
2:A:802:THR:HG23	2:E:609:LEU:O	2.16	0.45
2:B:827:TRP:CD1	2:B:828:GLN:N	2.85	0.45
1:G:76:ILE:HD13	1:G:82:MET:HG2	1.99	0.45
1:D:125:GLU:OE2	1:D:362:TYR:OH	2.34	0.45
2:E:833:VAL:HG23	2:E:915:PHE:HB3	1.99	0.45
2:E:740:LEU:HB2	2:E:884:LEU:HD13	1.98	0.45
1:D:341:ILE:HG22	1:D:345:ILE:HD12	1.97	0.45
2:C:656:ARG:HB3	2:C:661:ILE:HG13	1.99	0.45
2:A:609:LEU:C	2:A:610:PHE:HD1	2.20	0.45
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.98	0.45
1:H:295:ALA:O	1:H:328:LYS:HB3	2.16	0.45
1:D:8:LEU:HD11	1:D:94:LEU:CD1	2.46	0.45
2:E:603:LEU:O	2:E:606:PHE:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:VAL:HG23	1:H:33:SER:HB3	1.98	0.45
2:B:825:ASN:HB2	2:B:828:GLN:OE1	2.17	0.45
1:D:291:LYS:NZ	1:D:326:LYS:H	2.14	0.45
2:A:737:GLN:O	2:A:741:GLN:HG2	2.17	0.45
1:G:158:GLY:HA3	1:G:183:ARG:NH2	2.32	0.45
1:G:18:LYS:HG3	1:G:30:VAL:HG22	1.98	0.45
2:E:814:LEU:HG	2:E:932:ASN:ND2	2.32	0.45
1:H:116:ARG:HG3	1:H:134:VAL:HG11	1.99	0.45
2:E:877:ASN:O	2:E:880:LYS:N	2.50	0.45
2:B:761:GLN:CD	2:B:761:GLN:H	2.17	0.45
1:F:25:ASP:N	3:F:402:ACT:OXT	2.50	0.45
2:B:722:ARG:CZ	2:B:722:ARG:HA	2.46	0.45
1:D:316:GLU:O	1:D:320:LEU:HD13	2.17	0.45
1:H:99:GLU:O	1:H:130:PRO:HD3	2.17	0.45
2:B:656:ARG:HB3	2:B:661:ILE:HG13	1.98	0.45
2:B:673:LEU:HA	2:B:674:PRO:HD3	1.75	0.45
1:D:10:CYS:O	1:D:105:LEU:HA	2.17	0.45
1:H:316:GLU:O	1:H:320:LEU:HD13	2.17	0.45
1:H:341:ILE:HG22	1:H:345:ILE:HD12	1.99	0.45
2:A:584:ILE:HD11	2:E:787:GLY:HA3	1.98	0.45
2:E:599:GLU:O	2:E:601:LEU:HD12	2.17	0.45
2:E:746:GLN:NE2	1:G:323:SER:HB3	2.29	0.45
1:G:304:THR:O	1:G:335:ARG:NH2	2.44	0.45
1:D:333:PRO:HG2	1:D:334:GLU:HG3	1.98	0.45
1:H:288:ASP:OD1	1:H:288:ASP:N	2.50	0.45
1:D:350:SER:O	1:D:353:GLN:HG2	2.17	0.45
1:F:112:PRO:HD2	1:F:115:ASN:HB2	1.99	0.44
1:F:217:CYS:HB2	1:F:254:ARG:O	2.17	0.44
2:C:827:TRP:NE1	2:C:828:GLN:HG3	2.32	0.44
2:E:682:MET:O	2:E:685:LEU:HD12	2.17	0.44
2:C:738:ASP:O	2:C:741:GLN:HB2	2.16	0.44
1:H:118:LYS:O	1:H:122:ILE:HG13	2.17	0.44
1:F:147:ARG:NH1	1:F:330:ILE:HG12	2.21	0.44
2:A:603:LEU:O	2:A:606:PHE:HB3	2.17	0.44
1:G:105:LEU:HD13	1:G:134:VAL:HG22	1.99	0.44
2:C:581:PRO:HA	2:C:584:ILE:HB	1.99	0.44
2:C:669:ASP:HB2	2:C:730:MET:SD	2.57	0.44
1:D:362:TYR:O	1:D:366:GLY:N	2.40	0.44
1:G:172:PRO:O	1:G:175:ILE:HG13	2.17	0.44
1:F:288:ASP:OD1	1:F:288:ASP:N	2.50	0.44
2:C:707:LEU:HA	2:C:707:LEU:HD23	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:HIS:CD2	1:G:276:GLU:HG3	2.53	0.44
2:E:913:VAL:HG23	2:E:914:PHE:N	2.33	0.44
2:B:737:GLN:O	2:B:741:GLN:HG2	2.17	0.44
1:G:219:VAL:HG22	1:G:258:PRO:HB2	1.99	0.44
1:H:172:PRO:O	1:H:175:ILE:HG13	2.16	0.44
1:H:120:THR:HG21	1:H:370:VAL:HB	2.00	0.44
2:B:707:LEU:HD23	2:B:707:LEU:HA	1.84	0.44
2:B:789:LYS:HB3	2:B:791:GLN:OE1	2.18	0.44
1:H:105:LEU:HD13	1:H:134:VAL:HG22	2.00	0.44
1:F:52:SER:OG	1:F:84:LYS:HD2	2.18	0.44
1:G:109:PRO:O	1:G:110:LEU:HB2	2.17	0.44
1:H:124:PHE:HD1	1:H:359:LYS:HG3	1.83	0.44
2:A:874:LEU:HD23	2:A:878:GLU:HG3	2.00	0.44
1:D:25:ASP:HB3	3:D:401:ACT:O	2.17	0.44
2:E:669:ASP:HB2	2:E:730:MET:SD	2.58	0.44
2:B:646:ASN:HB3	1:H:148:THR:HG21	1.99	0.44
2:C:647:LEU:HD22	2:C:651:LEU:HG	1.99	0.44
1:D:365:ALA:HB3	1:D:369:ILE:HB	2.00	0.44
2:A:599:GLU:O	2:A:601:LEU:HD12	2.17	0.44
1:H:76:ILE:HD13	1:H:82:MET:HG2	2.00	0.44
2:A:807:THR:HG22	2:A:810:HIS:ND1	2.33	0.44
2:C:677:PHE:CZ	2:C:681:LEU:HD13	2.53	0.44
2:B:649:ILE:HD13	1:H:143:TYR:CE1	2.53	0.44
2:E:574:PHE:CE2	2:E:576:TRP:HB3	2.52	0.44
1:F:89:THR:O	1:F:94:LEU:HB2	2.17	0.44
2:C:669:ASP:HB3	2:C:673:LEU:CB	2.47	0.44
1:D:276:GLU:O	1:D:279:TYR:N	2.51	0.44
2:C:722:ARG:CZ	2:C:722:ARG:HA	2.47	0.44
2:E:581:PRO:HA	2:E:584:ILE:HB	2.00	0.44
2:A:790:LEU:HG	2:A:917:VAL:HG11	2.00	0.44
1:F:73:HIS:HB3	1:F:177:ARG:NH2	2.32	0.43
1:F:99:GLU:O	1:F:130:PRO:HD3	2.18	0.43
2:B:581:PRO:HA	2:B:584:ILE:HB	2.01	0.43
2:C:609:LEU:C	2:C:610:PHE:HD1	2.21	0.43
2:A:669:ASP:HB3	2:A:673:LEU:CB	2.45	0.43
1:D:105:LEU:O	1:D:134:VAL:HA	2.18	0.43
1:F:352:PHE:HA	1:F:355:MET:HE2	2.00	0.43
2:C:682:MET:O	2:C:685:LEU:HD12	2.18	0.43
1:F:178:LEU:HG	1:F:180:LEU:H	1.82	0.43
1:F:6:THR:O	1:F:101:HIS:HB3	2.16	0.43
1:F:275:HIS:CD2	1:F:276:GLU:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:695:ARG:HG3	2:A:696:GLN:H	1.83	0.43
1:D:261:LEU:HB3	1:D:274:ILE:CD1	2.37	0.43
2:B:682:MET:O	2:B:685:LEU:HD12	2.18	0.43
2:E:874:LEU:HD23	2:E:878:GLU:HG3	2.01	0.43
2:C:874:LEU:HD23	2:C:878:GLU:HG3	2.01	0.43
2:C:905:SER:O	2:C:909:THR:N	2.50	0.43
1:G:73:HIS:HB3	1:G:177:ARG:NH2	2.33	0.43
1:F:242:LEU:HB2	1:F:246:GLN:O	2.18	0.43
2:B:796:LEU:HD23	2:B:796:LEU:HA	1.68	0.43
2:E:576:TRP:CD1	2:E:576:TRP:O	2.69	0.43
1:G:341:ILE:HG22	1:G:345:ILE:HD12	2.00	0.43
2:E:773:LEU:HA	2:E:773:LEU:HD12	1.82	0.43
2:C:599:GLU:O	2:C:601:LEU:HD12	2.18	0.43
2:E:606:PHE:HE1	2:E:610:PHE:CD2	2.37	0.43
2:B:576:TRP:CD1	2:B:576:TRP:O	2.68	0.43
1:D:73:HIS:HB3	1:D:177:ARG:NH2	2.33	0.43
2:A:840:SER:O	2:A:844:VAL:HG23	2.18	0.43
1:H:300:SER:HB2	1:H:338:SER:HB2	2.01	0.43
2:C:842:GLU:O	2:C:846:LEU:HG	2.18	0.43
1:H:274:ILE:HG21	1:H:313:MET:HE1	2.00	0.43
1:H:111:ASN:HD21	1:H:115:ASN:CG	2.15	0.43
1:D:94:LEU:HD22	1:D:94:LEU:HA	1.76	0.43
1:D:148:THR:HG21	2:A:646:ASN:HB3	2.00	0.43
2:E:678:VAL:O	2:E:682:MET:HG3	2.19	0.43
1:F:109:PRO:HG2	1:F:161:HIS:CG	2.54	0.43
1:F:27:PRO:HD3	1:F:340:TRP:CD2	2.54	0.43
1:D:264:PRO:CG	1:D:273:GLY:HA2	2.49	0.43
1:H:362:TYR:O	1:H:366:GLY:N	2.42	0.43
2:B:894:ALA:O	2:B:897:ALA:HB3	2.19	0.43
2:A:656:ARG:HB3	2:A:661:ILE:HG13	2.00	0.43
1:H:112:PRO:HD2	1:H:115:ASN:HB2	2.01	0.42
2:B:690:GLU:O	2:B:694:LEU:HD23	2.18	0.42
2:E:645:LYS:HE3	2:E:645:LYS:HB3	1.74	0.42
2:A:842:GLU:O	2:A:846:LEU:HG	2.19	0.42
2:A:637:THR:HG22	2:A:639:LEU:N	2.28	0.42
2:C:779:SER:C	2:C:781:LYS:H	2.23	0.42
2:E:690:GLU:O	2:E:694:LEU:HD23	2.19	0.42
1:H:188:TYR:HH	1:H:266:PHE:HD2	1.65	0.42
2:B:677:PHE:CZ	2:B:681:LEU:HD13	2.54	0.42
2:C:782:ARG:NH1	2:B:573:VAL:HG23	2.34	0.42
1:F:291:LYS:NZ	1:F:326:LYS:H	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:GLU:O	1:F:320:LEU:HD13	2.19	0.42
2:C:816:VAL:HG11	2:C:925:TYR:OH	2.18	0.42
2:C:704:LEU:HA	2:C:704:LEU:HD13	1.77	0.42
1:H:210:ARG:O	1:H:213:LYS:HB3	2.20	0.42
2:B:645:LYS:HB3	2:B:645:LYS:HE3	1.71	0.42
2:A:707:LEU:HD22	2:A:711:ASP:HB2	2.01	0.42
1:F:295:ALA:O	1:F:328:LYS:HB3	2.19	0.42
1:G:313:MET:O	1:G:317:ILE:HG12	2.19	0.42
1:D:136:ILE:H	1:D:136:ILE:CD1	2.25	0.42
1:G:350:SER:O	1:G:353:GLN:HG2	2.20	0.42
1:F:321:ALA:HB3	1:F:327:ILE:HD11	2.01	0.42
1:H:361:GLU:H	1:H:361:GLU:HG2	1.53	0.42
1:D:176:MET:HG3	1:D:281:SER:HB2	2.01	0.42
1:F:31:PHE:HZ	1:F:89:THR:HG1	1.66	0.42
1:H:109:PRO:O	1:H:110:LEU:HB2	2.20	0.42
1:D:92:ASN:O	1:D:95:ARG:HD2	2.20	0.42
2:C:574:PHE:CE2	2:C:576:TRP:HB3	2.55	0.42
2:A:678:VAL:O	2:A:682:MET:HG3	2.20	0.42
1:F:361:GLU:H	1:F:361:GLU:HG2	1.54	0.42
1:D:120:THR:HG21	1:D:370:VAL:HB	2.01	0.42
1:F:274:ILE:HG21	1:F:313:MET:HE1	2.00	0.42
2:A:576:TRP:CD1	2:A:576:TRP:O	2.71	0.42
1:G:196:ARG:HH21	1:G:251:GLY:N	2.17	0.42
2:E:747:LEU:HD23	2:E:747:LEU:HA	1.79	0.42
1:H:372:ARG:HG2	1:H:372:ARG:H	1.68	0.42
2:C:576:TRP:O	2:C:576:TRP:CD1	2.70	0.42
2:E:673:LEU:HA	2:E:674:PRO:HD3	1.78	0.42
2:E:646:ASN:HB3	2:E:684:PHE:HZ	1.83	0.42
1:D:275:HIS:CD2	1:D:276:GLU:HG3	2.54	0.42
1:G:264:PRO:CG	1:G:273:GLY:HA2	2.49	0.42
1:F:365:ALA:HB3	1:F:369:ILE:HB	2.02	0.42
1:D:219:VAL:HG22	1:D:258:PRO:HB2	2.00	0.42
2:C:894:ALA:O	2:C:897:ALA:HB3	2.20	0.42
2:B:816:VAL:HG11	2:B:925:TYR:OH	2.20	0.42
1:G:146:GLY:C	1:G:147:ARG:HG2	2.40	0.42
2:E:609:LEU:C	2:E:610:PHE:HD1	2.23	0.42
1:H:109:PRO:HG2	1:H:161:HIS:CG	2.54	0.42
1:H:111:ASN:HA	1:H:112:PRO:HD3	1.69	0.42
2:A:645:LYS:HE3	2:A:645:LYS:HB3	1.72	0.42
2:A:899:VAL:HG22	2:A:914:PHE:CD1	2.55	0.42
2:A:863:SER:HB2	2:C:582:ASN:ND2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:796:LEU:HD23	2:C:796:LEU:HA	1.57	0.42
2:E:576:TRP:CD1	2:E:576:TRP:C	2.94	0.41
2:A:581:PRO:HA	2:A:584:ILE:HB	2.02	0.41
1:F:315:LYS:HG3	1:F:316:GLU:N	2.35	0.41
1:F:120:THR:HG21	1:F:370:VAL:HB	2.02	0.41
1:G:365:ALA:HB3	1:G:369:ILE:HB	2.01	0.41
1:F:206:ARG:HA	1:F:209:VAL:HG23	2.02	0.41
2:B:565:ILE:HG23	2:B:566:LYS:N	2.33	0.41
1:H:217:CYS:HB2	1:H:254:ARG:O	2.19	0.41
2:E:646:ASN:HB3	1:G:148:THR:HG21	2.02	0.41
1:D:314:GLN:O	1:D:318:THR:OG1	2.38	0.41
1:D:99:GLU:O	1:D:130:PRO:HD3	2.20	0.41
1:G:288:ASP:OD1	1:G:288:ASP:N	2.52	0.41
1:G:311:ASP:O	1:G:314:GLN:HB3	2.20	0.41
2:E:789:LYS:HB3	2:E:791:GLN:OE1	2.20	0.41
1:H:151:ILE:HD11	1:H:162:ASN:HB3	2.01	0.41
1:H:94:LEU:HA	1:H:94:LEU:HD22	1.85	0.41
2:C:790:LEU:HD12	2:C:790:LEU:HA	1.90	0.41
2:A:588:VAL:O	2:A:591:GLU:HB2	2.20	0.41
1:F:158:GLY:HA3	1:F:183:ARG:NH2	2.34	0.41
2:C:576:TRP:C	2:C:576:TRP:CD1	2.93	0.41
1:F:173:HIS:H	1:F:173:HIS:CD2	2.35	0.41
2:E:812:ILE:HG13	2:E:812:ILE:H	1.67	0.41
2:C:779:SER:HA	2:C:783:GLY:O	2.21	0.41
2:E:677:PHE:CZ	2:E:681:LEU:HD13	2.56	0.41
2:E:910:PRO:HD2	2:E:913:VAL:HG22	2.03	0.41
2:C:678:VAL:O	2:C:682:MET:HG3	2.20	0.41
2:B:603:LEU:O	2:B:606:PHE:HB3	2.20	0.41
2:E:588:VAL:O	2:E:591:GLU:HB2	2.20	0.41
1:G:120:THR:HG21	1:G:370:VAL:HB	2.00	0.41
2:B:672:THR:O	2:B:672:THR:OG1	2.17	0.41
1:G:92:ASN:O	1:G:95:ARG:HD2	2.21	0.41
1:D:302:GLY:O	4:D:402:ATP:C4	2.74	0.41
2:C:565:ILE:HG23	2:C:566:LYS:N	2.36	0.41
2:B:774:GLY:O	2:B:778:ASN:HB2	2.19	0.41
2:A:587:THR:HB	2:E:901:TYR:O	2.21	0.41
2:A:584:ILE:O	2:A:587:THR:HG23	2.20	0.41
2:C:790:LEU:HG	2:C:917:VAL:HG11	2.03	0.41
1:H:347:ALA:HA	1:H:352:PHE:CE2	2.56	0.41
1:D:17:VAL:HG23	1:D:33:SER:HB3	2.02	0.41
1:G:321:ALA:HB3	1:G:327:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:842:GLU:O	2:E:846:LEU:HG	2.20	0.41
2:E:704:LEU:HA	2:E:704:LEU:HD13	1.85	0.41
2:A:747:LEU:HD23	2:A:747:LEU:HA	1.73	0.41
2:B:850:GLU:O	2:B:853:ARG:HG3	2.21	0.41
1:G:261:LEU:HB3	1:G:274:ILE:CD1	2.38	0.41
1:D:173:HIS:H	1:D:173:HIS:CD2	2.35	0.41
2:E:757:VAL:HA	2:E:830:LEU:CD2	2.48	0.41
2:A:606:PHE:HE1	2:A:610:PHE:CD2	2.38	0.41
2:B:651:LEU:O	2:B:654:ALA:HB3	2.20	0.41
2:A:913:VAL:HG23	2:A:914:PHE:N	2.35	0.41
1:F:287:ILE:HG23	1:F:290:ARG:HH12	1.85	0.41
1:G:109:PRO:HG2	1:G:161:HIS:CG	2.55	0.41
1:G:314:GLN:O	1:G:318:THR:OG1	2.36	0.41
2:B:807:THR:HG22	2:B:810:HIS:CG	2.56	0.41
1:D:18:LYS:HG3	1:D:30:VAL:HG22	2.03	0.41
2:B:687:THR:O	2:B:691:VAL:HG23	2.21	0.41
1:H:321:ALA:HB3	1:H:327:ILE:HD11	2.02	0.41
1:G:118:LYS:O	1:G:122:ILE:HG13	2.20	0.41
2:E:756:SER:HB2	2:E:830:LEU:HA	2.03	0.41
1:H:21:PHE:HB2	3:H:401:ACT:H3	2.03	0.41
2:C:672:THR:O	2:C:674:PRO:HD3	2.21	0.41
2:E:672:THR:O	2:E:674:PRO:HD3	2.21	0.41
2:B:856:GLU:HA	2:B:859:ARG:HG2	2.03	0.41
1:F:18:LYS:HG3	1:F:30:VAL:HG22	2.01	0.41
1:G:242:LEU:HB2	1:G:246:GLN:O	2.20	0.41
2:E:652:ARG:NE	1:G:345:ILE:HG12	2.36	0.41
2:B:842:GLU:O	2:B:846:LEU:HG	2.21	0.41
2:E:816:VAL:HG11	2:E:925:TYR:OH	2.21	0.41
2:E:645:LYS:HG2	2:E:649:ILE:HD11	2.03	0.41
1:H:264:PRO:CG	1:H:273:GLY:HA2	2.51	0.41
2:A:877:ASN:O	2:A:880:LYS:N	2.54	0.41
1:G:173:HIS:H	1:G:173:HIS:CD2	2.35	0.40
1:D:151:ILE:HD11	1:D:162:ASN:HB3	2.03	0.40
1:H:162:ASN:O	1:H:164:PRO:HD3	2.20	0.40
2:C:673:LEU:HA	2:C:674:PRO:HD3	1.79	0.40
1:G:196:ARG:NH1	1:G:196:ARG:HB3	2.35	0.40
1:F:105:LEU:HD13	1:F:134:VAL:HG22	2.03	0.40
1:G:257:CYS:HB3	1:G:258:PRO:HD3	2.03	0.40
1:H:208:ILE:O	1:H:212:ILE:HD12	2.20	0.40
2:C:610:PHE:CE2	2:B:808:LEU:HA	2.56	0.40
2:A:856:GLU:HA	2:A:859:ARG:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:814:LEU:HG	2:A:932:ASN:ND2	2.35	0.40
2:B:678:VAL:O	2:B:682:MET:HG3	2.22	0.40
1:D:102:PRO:HB3	1:D:131:ALA:HB3	2.03	0.40
1:H:365:ALA:HB3	1:H:369:ILE:HB	2.03	0.40
2:A:796:LEU:HD23	2:A:796:LEU:HA	1.65	0.40
2:B:779:SER:C	2:B:781:LYS:H	2.24	0.40
1:F:287:ILE:H	1:F:287:ILE:HG12	1.65	0.40
1:D:160:THR:HB	1:D:178:LEU:HB3	2.03	0.40
2:B:584:ILE:HD13	2:B:584:ILE:HA	1.95	0.40
1:F:124:PHE:HD1	1:F:359:LYS:HG3	1.86	0.40
2:A:770:ILE:HG22	2:A:788:PHE:CE2	2.57	0.40
2:A:669:ASP:HB2	2:A:730:MET:SD	2.61	0.40
2:A:609:LEU:O	2:E:802:THR:HG23	2.20	0.40
1:H:257:CYS:HB3	1:H:258:PRO:HD3	2.04	0.40
1:H:209:VAL:HA	1:H:212:ILE:HD13	2.03	0.40
1:D:123:MET:HG3	1:D:132:MET:HE3	2.02	0.40
1:F:210:ARG:O	1:F:213:LYS:HB3	2.21	0.40
1:D:361:GLU:H	1:D:361:GLU:HG2	1.51	0.40
2:E:803:ASP:OD2	2:E:805:LYS:HB2	2.22	0.40
1:D:106:THR:HA	1:D:135:ALA:O	2.21	0.40
2:A:913:VAL:C	2:A:916:PRO:HD2	2.42	0.40
2:E:774:GLY:O	2:E:778:ASN:HB2	2.22	0.40
2:B:773:LEU:HD21	2:B:811:PHE:CE2	2.56	0.40
1:H:304:THR:O	1:H:335:ARG:NH2	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:SER:OG	1:F:62:ARG:O[1_554]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	352/377 (93%)	326 (93%)	25 (7%)	1 (0%)	46	82
1	F	352/377 (93%)	324 (92%)	27 (8%)	1 (0%)	46	82
1	G	352/377 (93%)	324 (92%)	27 (8%)	1 (0%)	46	82
1	H	352/377 (93%)	325 (92%)	26 (7%)	1 (0%)	46	82
2	A	353/402 (88%)	310 (88%)	37 (10%)	6 (2%)	11	51
2	B	353/402 (88%)	313 (89%)	34 (10%)	6 (2%)	11	51
2	C	353/402 (88%)	313 (89%)	34 (10%)	6 (2%)	11	51
2	E	353/402 (88%)	310 (88%)	38 (11%)	5 (1%)	14	55
All	All	2820/3116 (90%)	2545 (90%)	248 (9%)	27 (1%)	19	63

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	869	VAL
2	E	869	VAL
2	C	869	VAL
2	B	869	VAL
2	A	598	LEU
2	A	674	PRO
2	E	598	LEU
2	E	674	PRO
2	C	598	LEU
2	C	674	PRO
2	B	598	LEU
2	B	674	PRO
2	C	826	PHE
2	A	826	PHE
2	A	863	SER
2	E	826	PHE
2	E	863	SER
2	C	863	SER
2	B	695	ARG
2	B	826	PHE
2	B	863	SER
2	A	752	ALA
2	C	695	ARG
1	D	274	ILE
1	F	274	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	274	ILE
1	H	274	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	302/320 (94%)	262 (87%)	40 (13%)	5	25
1	F	302/320 (94%)	260 (86%)	42 (14%)	4	23
1	G	302/320 (94%)	263 (87%)	39 (13%)	5	26
1	H	302/320 (94%)	265 (88%)	37 (12%)	6	28
2	A	316/351 (90%)	256 (81%)	60 (19%)	2	9
2	B	316/351 (90%)	255 (81%)	61 (19%)	2	8
2	C	316/351 (90%)	254 (80%)	62 (20%)	1	8
2	E	316/351 (90%)	256 (81%)	60 (19%)	2	9
All	All	2472/2684 (92%)	2071 (84%)	401 (16%)	3	16

All (401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	6	THR
1	D	18	LYS
1	D	28	ARG
1	D	57	GLU
1	D	66	THR
1	D	69	TYR
1	D	71	ILE
1	D	78	ASN
1	D	94	LEU
1	D	95	ARG
1	D	99	GLU
1	D	101	HIS
1	D	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	119	MET
1	D	120	THR
1	D	136	ILE
1	D	151	ILE
1	D	159	VAL
1	D	176	MET
1	D	179	ASP
1	D	200	PHE
1	D	202	THR
1	D	217	CYS
1	D	277	THR
1	D	280	ASN
1	D	288	ASP
1	D	289	ILE
1	D	290	ARG
1	D	292	ASP
1	D	315	LYS
1	D	318	THR
1	D	326	LYS
1	D	334	GLU
1	D	338	SER
1	D	339	VAL
1	D	349	LEU
1	D	360	GLN
1	D	368	SER
1	D	370	VAL
1	D	372	ARG
2	A	565	ILE
2	A	576	TRP
2	A	577	THR
2	A	585	ASN
2	A	587	THR
2	A	591	GLU
2	A	592	LEU
2	A	594	ASP
2	A	598	LEU
2	A	601	LEU
2	A	603	LEU
2	A	609	LEU
2	A	613	LYS
2	A	636	VAL
2	A	640	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	643	ARG
2	A	647	LEU
2	A	669	ASP
2	A	675	VAL
2	A	685	LEU
2	A	700	GLU
2	A	701	ARG
2	A	705	GLU
2	A	711	ASP
2	A	721	GLU
2	A	722	ARG
2	A	724	THR
2	A	725	GLN
2	A	738	ASP
2	A	740	LEU
2	A	742	MET
2	A	750	ILE
2	A	751	ILE
2	A	754	SER
2	A	764	LYS
2	A	765	GLN
2	A	775	ASN
2	A	781	LYS
2	A	792	SER
2	A	795	LEU
2	A	798	ASP
2	A	802	THR
2	A	808	LEU
2	A	810	HIS
2	A	815	THR
2	A	816	VAL
2	A	822	GLU
2	A	825	ASN
2	A	826	PHE
2	A	830	LEU
2	A	841	LEU
2	A	853	ARG
2	A	865	HIS
2	A	869	VAL
2	A	876	THR
2	A	882	ASP
2	A	886	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	898	VAL
2	A	909	THR
2	A	925	TYR
2	E	565	ILE
2	E	576	TRP
2	E	577	THR
2	E	585	ASN
2	E	587	THR
2	E	591	GLU
2	E	592	LEU
2	E	594	ASP
2	E	598	LEU
2	E	601	LEU
2	E	603	LEU
2	E	609	LEU
2	E	613	LYS
2	E	636	VAL
2	E	640	GLU
2	E	643	ARG
2	E	647	LEU
2	E	669	ASP
2	E	675	VAL
2	E	685	LEU
2	E	693	LEU
2	E	700	GLU
2	E	701	ARG
2	E	705	GLU
2	E	711	ASP
2	E	721	GLU
2	E	722	ARG
2	E	724	THR
2	E	725	GLN
2	E	738	ASP
2	E	740	LEU
2	E	742	MET
2	E	750	ILE
2	E	751	ILE
2	E	764	LYS
2	E	765	GLN
2	E	775	ASN
2	E	781	LYS
2	E	792	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	795	LEU
2	E	798	ASP
2	E	802	THR
2	E	808	LEU
2	E	810	HIS
2	E	815	THR
2	E	816	VAL
2	E	822	GLU
2	E	825	ASN
2	E	826	PHE
2	E	830	LEU
2	E	841	LEU
2	E	853	ARG
2	E	865	HIS
2	E	869	VAL
2	E	876	THR
2	E	882	ASP
2	E	886	ARG
2	E	898	VAL
2	E	909	THR
2	E	925	TYR
2	C	565	ILE
2	C	576	TRP
2	C	577	THR
2	C	585	ASN
2	C	587	THR
2	C	591	GLU
2	C	592	LEU
2	C	594	ASP
2	C	598	LEU
2	C	601	LEU
2	C	603	LEU
2	C	609	LEU
2	C	613	LYS
2	C	636	VAL
2	C	640	GLU
2	C	643	ARG
2	C	647	LEU
2	C	669	ASP
2	C	675	VAL
2	C	685	LEU
2	C	693	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	700	GLU
2	C	701	ARG
2	C	704	LEU
2	C	705	GLU
2	C	711	ASP
2	C	721	GLU
2	C	722	ARG
2	C	724	THR
2	C	725	GLN
2	C	738	ASP
2	C	740	LEU
2	C	742	MET
2	C	750	ILE
2	C	751	ILE
2	C	754	SER
2	C	764	LYS
2	C	765	GLN
2	C	775	ASN
2	C	781	LYS
2	C	792	SER
2	C	795	LEU
2	C	798	ASP
2	C	802	THR
2	C	808	LEU
2	C	810	HIS
2	C	815	THR
2	C	816	VAL
2	C	822	GLU
2	C	825	ASN
2	C	826	PHE
2	C	830	LEU
2	C	841	LEU
2	C	853	ARG
2	C	865	HIS
2	C	869	VAL
2	C	876	THR
2	C	882	ASP
2	C	886	ARG
2	C	898	VAL
2	C	909	THR
2	C	925	TYR
2	B	565	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	576	TRP
2	B	577	THR
2	B	585	ASN
2	B	587	THR
2	B	591	GLU
2	B	592	LEU
2	B	594	ASP
2	B	598	LEU
2	B	601	LEU
2	B	603	LEU
2	B	609	LEU
2	B	613	LYS
2	B	636	VAL
2	B	640	GLU
2	B	643	ARG
2	B	647	LEU
2	B	669	ASP
2	B	675	VAL
2	B	685	LEU
2	B	693	LEU
2	B	700	GLU
2	B	701	ARG
2	B	705	GLU
2	B	711	ASP
2	B	721	GLU
2	B	722	ARG
2	B	724	THR
2	B	725	GLN
2	B	738	ASP
2	B	740	LEU
2	B	742	MET
2	B	750	ILE
2	B	751	ILE
2	B	754	SER
2	B	764	LYS
2	B	765	GLN
2	B	775	ASN
2	B	781	LYS
2	B	792	SER
2	B	795	LEU
2	B	798	ASP
2	B	802	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	808	LEU
2	B	810	HIS
2	B	815	THR
2	B	816	VAL
2	B	822	GLU
2	B	825	ASN
2	B	826	PHE
2	B	830	LEU
2	B	841	LEU
2	B	853	ARG
2	B	865	HIS
2	B	869	VAL
2	B	876	THR
2	B	882	ASP
2	B	886	ARG
2	B	898	VAL
2	B	909	THR
2	B	925	TYR
1	H	6	THR
1	H	18	LYS
1	H	57	GLU
1	H	69	TYR
1	H	71	ILE
1	H	78	ASN
1	H	94	LEU
1	H	95	ARG
1	H	99	GLU
1	H	101	HIS
1	H	105	LEU
1	H	119	MET
1	H	120	THR
1	H	136	ILE
1	H	151	ILE
1	H	159	VAL
1	H	176	MET
1	H	179	ASP
1	H	200	PHE
1	H	202	THR
1	H	217	CYS
1	H	277	THR
1	H	280	ASN
1	H	288	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	290	ARG
1	H	292	ASP
1	H	315	LYS
1	H	318	THR
1	H	326	LYS
1	H	334	GLU
1	H	338	SER
1	H	339	VAL
1	H	349	LEU
1	H	360	GLN
1	H	368	SER
1	H	370	VAL
1	H	372	ARG
1	G	6	THR
1	G	18	LYS
1	G	57	GLU
1	G	69	TYR
1	G	71	ILE
1	G	78	ASN
1	G	94	LEU
1	G	95	ARG
1	G	99	GLU
1	G	101	HIS
1	G	105	LEU
1	G	119	MET
1	G	120	THR
1	G	136	ILE
1	G	147	ARG
1	G	151	ILE
1	G	159	VAL
1	G	176	MET
1	G	179	ASP
1	G	200	PHE
1	G	202	THR
1	G	217	CYS
1	G	229	THR
1	G	277	THR
1	G	280	ASN
1	G	288	ASP
1	G	290	ARG
1	G	292	ASP
1	G	315	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	318	THR
1	G	326	LYS
1	G	334	GLU
1	G	338	SER
1	G	339	VAL
1	G	349	LEU
1	G	360	GLN
1	G	368	SER
1	G	370	VAL
1	G	372	ARG
1	F	6	THR
1	F	18	LYS
1	F	28	ARG
1	F	57	GLU
1	F	66	THR
1	F	69	TYR
1	F	71	ILE
1	F	78	ASN
1	F	94	LEU
1	F	95	ARG
1	F	99	GLU
1	F	101	HIS
1	F	105	LEU
1	F	119	MET
1	F	120	THR
1	F	136	ILE
1	F	147	ARG
1	F	151	ILE
1	F	159	VAL
1	F	176	MET
1	F	179	ASP
1	F	200	PHE
1	F	202	THR
1	F	217	CYS
1	F	229	THR
1	F	277	THR
1	F	280	ASN
1	F	288	ASP
1	F	290	ARG
1	F	292	ASP
1	F	315	LYS
1	F	318	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	326	LYS
1	F	334	GLU
1	F	338	SER
1	F	339	VAL
1	F	349	LEU
1	F	351	THR
1	F	360	GLN
1	F	368	SER
1	F	370	VAL
1	F	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	101	HIS
1	D	137	GLN
2	A	746	GLN
2	E	746	GLN
2	C	746	GLN
2	B	746	GLN
1	H	101	HIS
1	G	101	HIS
1	F	101	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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	ACT	A	1001	-	1,3,3	0.35	0	0,3,3	0.00	-
3	ACT	A	1002	-	1,3,3	1.64	0	0,3,3	0.00	-
3	ACT	A	1003	-	1,3,3	1.60	0	0,3,3	0.00	-
3	ACT	B	1001	-	1,3,3	1.12	0	0,3,3	0.00	-
3	ACT	C	1001	-	1,3,3	0.70	0	0,3,3	0.00	-
3	ACT	C	1002	-	1,3,3	2.15	1 (100%)	0,3,3	0.00	-
3	ACT	D	401	-	1,3,3	0.63	0	0,3,3	0.00	-
4	ATP	D	402	-	24,33,33	0.88	1 (4%)	31,52,52	1.92	5 (16%)
3	ACT	E	1001	-	1,3,3	1.85	0	0,3,3	0.00	-
3	ACT	F	401	-	1,3,3	1.63	0	0,3,3	0.00	-
3	ACT	F	402	-	1,3,3	1.29	0	0,3,3	0.00	-
4	ATP	F	403	-	24,33,33	0.90	1 (4%)	31,52,52	1.83	4 (12%)
3	ACT	G	401	-	1,3,3	0.51	0	0,3,3	0.00	-
4	ATP	G	402	-	24,33,33	1.05	2 (8%)	31,52,52	1.68	6 (19%)
3	ACT	H	401	-	1,3,3	0.92	0	0,3,3	0.00	-
4	ATP	H	402	-	24,33,33	1.16	3 (12%)	31,52,52	1.47	4 (12%)

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	ACT	A	1001	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1003	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1001	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1001	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	D	401	-	-	0/0/0/0	0/0/0/0
4	ATP	D	402	-	-	0/18/38/38	0/3/3/3
3	ACT	E	1001	-	-	0/0/0/0	0/0/0/0
3	ACT	F	401	-	-	0/0/0/0	0/0/0/0
3	ACT	F	402	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	F	403	-	-	0/18/38/38	0/3/3/3
3	ACT	G	401	-	-	0/0/0/0	0/0/0/0
4	ATP	G	402	-	-	0/18/38/38	0/3/3/3
3	ACT	H	401	-	-	0/0/0/0	0/0/0/0
4	ATP	H	402	-	-	0/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	402	ATP	C2-N3	2.03	1.35	1.32
4	G	402	ATP	O4'-C1'	2.06	1.43	1.41
3	C	1002	ACT	CH3-C	2.15	1.51	1.48
4	H	402	ATP	O4'-C1'	2.21	1.44	1.41
4	D	402	ATP	C5-C4	2.52	1.46	1.40
4	F	403	ATP	C5-C4	2.70	1.46	1.40
4	G	402	ATP	C5-C4	3.34	1.48	1.40
4	H	402	ATP	C5-C4	3.60	1.48	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	ATP	N3-C2-N1	-6.99	123.54	128.89
4	F	403	ATP	N3-C2-N1	-6.02	124.29	128.89
4	G	402	ATP	N3-C2-N1	-5.76	124.49	128.89
4	F	403	ATP	C2'-C1'-N9	-5.48	105.92	114.29
4	H	402	ATP	N3-C2-N1	-4.80	125.22	128.89
4	D	402	ATP	C4-C5-N7	-4.07	105.74	109.48
4	G	402	ATP	C4-C5-N7	-3.87	105.92	109.48
4	D	402	ATP	C1'-N9-C4	-3.84	121.14	126.94
4	H	402	ATP	C4-C5-N7	-2.72	106.98	109.48
4	H	402	ATP	O3'-C3'-C2'	-2.50	103.69	111.83
4	G	402	ATP	PA-O3A-PB	-2.44	125.88	132.73
4	F	403	ATP	C4-C5-N7	-2.42	107.25	109.48
4	F	403	ATP	PA-O3A-PB	-2.36	126.09	132.73
4	G	402	ATP	C1'-N9-C4	-2.27	123.52	126.94
4	G	402	ATP	PB-O3B-PG	-2.24	125.15	132.67
4	G	402	ATP	O4'-C1'-N9	2.00	112.29	108.10
4	D	402	ATP	C2-N1-C6	2.01	122.36	118.77
4	H	402	ATP	C2'-C3'-C4'	2.27	107.29	102.61
4	D	402	ATP	O3A-PA-O5'	3.00	110.89	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	ACT	1	0
3	B	1001	ACT	2	0
3	C	1001	ACT	1	0
3	C	1002	ACT	1	0
3	D	401	ACT	2	0
4	D	402	ATP	5	0
3	E	1001	ACT	1	0
3	F	402	ACT	1	0
4	F	403	ATP	1	0
3	G	401	ACT	2	0
4	G	402	ATP	2	0
3	H	401	ACT	2	0
4	H	402	ATP	2	0

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	D	356/377 (94%)	0.03	2 (0%) 90 86	58, 95, 163, 191	33 (9%)
1	F	356/377 (94%)	0.05	4 (1%) 82 77	59, 95, 164, 190	15 (4%)
1	G	356/377 (94%)	-0.11	1 (0%) 94 92	61, 97, 165, 192	33 (9%)
1	H	356/377 (94%)	-0.01	5 (1%) 78 73	64, 97, 164, 194	28 (7%)
2	A	357/402 (88%)	-0.17	1 (0%) 94 92	64, 101, 144, 163	61 (17%)
2	B	357/402 (88%)	-0.22	0 100 100	64, 102, 144, 165	59 (16%)
2	C	357/402 (88%)	-0.14	0 100 100	65, 102, 144, 160	56 (15%)
2	E	357/402 (88%)	-0.24	1 (0%) 94 92	65, 102, 143, 161	62 (17%)
All	All	2852/3116 (91%)	-0.10	14 (0%) 91 89	58, 99, 156, 194	347 (12%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	52	SER	3.7
1	F	239	SER	3.1
2	A	780	SER	2.9
1	H	199	SER	2.9
1	H	245	GLY	2.7
1	G	53	TYR	2.4
2	E	703	PRO	2.4
1	D	53	TYR	2.3
1	H	39	ARG	2.3
1	F	240	TYR	2.2
1	H	32	PRO	2.2
1	F	241	GLU	2.1
1	D	240	TYR	2.0
1	F	243	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	E	1001	4/4	0.92	0.54	6.55	73,103,103,103	0
3	ACT	F	401	4/4	0.79	0.45	5.02	88,111,123,124	0
3	ACT	H	401	4/4	0.94	0.34	1.41	70,89,100,122	0
3	ACT	F	402	4/4	0.90	0.27	0.98	78,80,106,107	0
3	ACT	D	401	4/4	0.97	0.26	0.49	62,66,91,110	0
3	ACT	G	401	4/4	0.97	0.26	0.43	84,88,105,122	0
3	ACT	A	1001	4/4	0.94	0.22	-0.25	72,74,83,89	0
3	ACT	C	1001	4/4	0.93	0.20	-0.29	75,88,90,100	0
4	ATP	H	402	31/31	0.95	0.17	-0.30	85,109,122,133	0
4	ATP	D	402	31/31	0.98	0.21	-0.31	53,86,104,106	0
3	ACT	A	1002	4/4	0.92	0.21	-0.36	80,96,99,103	0
4	ATP	G	402	31/31	0.96	0.19	-0.39	73,104,119,122	0
3	ACT	C	1002	4/4	0.89	0.21	-0.54	69,89,92,102	0
3	ACT	B	1001	4/4	0.93	0.17	-0.57	75,94,95,97	0
3	ACT	A	1003	4/4	0.95	0.18	-0.57	81,83,97,104	0
4	ATP	F	403	31/31	0.97	0.18	-0.57	70,91,110,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.