Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 12:32 PM EDT

PDB ID	:	6CHT
Title	:	HNF4alpha in complex with the corepressor EBP1 fragment
Authors	:	Chi, Y.I.; Singh, P.; Lee, I.K.
Deposited on	:	2018-02-22
Resolution	:	3.17 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

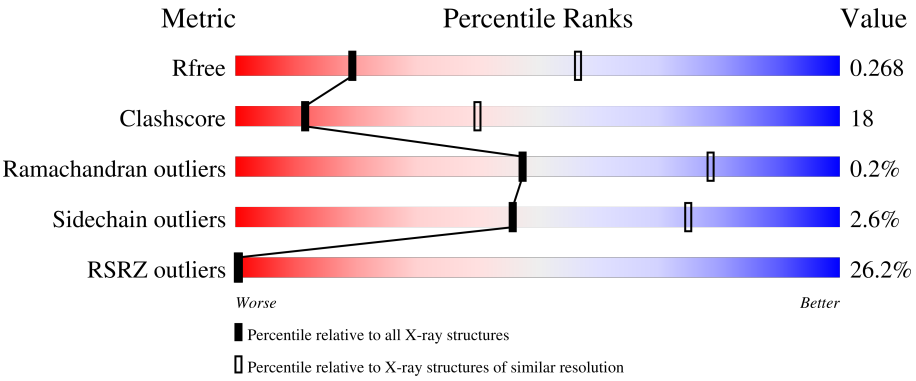
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.17 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}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	245	14% 53% 31% · 14%
1	B	245	8% 54% 29% 16%
1	D	245	18% 55% 30% · 13%
1	E	245	10% 53% 30% 17%
1	G	245	15% 52% 33% · 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	245	11% 45% 36% 18%
1	J	245	13% 48% 36% 15%
1	K	245	7% 51% 31% 18%
1	M	245	40% 48% 33% 18%
1	N	245	36% 42% 36% 21%
1	P	245	40% 42% 38% 18%
1	Q	245	35% 46% 33% 20%
1	S	245	25% 49% 31% 18%
1	T	245	24% 45% 32% 22%
1	V	245	29% 47% 34% 18%
1	W	245	23% 47% 30% 22%
2	C	20	5% 20% 15% 65%
2	F	20	5% 30% 5% 65%
2	I	20	10% 25% 10% 65%
2	L	20	15% 35% 5% 60%

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	DAO	D	500	-	-	-	X
3	DAO	G	500	-	-	-	X
3	DAO	H	500	-	-	-	X
3	DAO	J	500	-	-	-	X
3	DAO	K	500	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26381 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 Hepatocyte nuclear factor 4-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1681	1086	278	308	9			
1	B	205	Total	C	N	O	S	0	0	0
			1647	1062	275	301	9			
1	D	214	Total	C	N	O	S	0	0	0
			1712	1104	285	314	9			
1	E	204	Total	C	N	O	S	0	0	0
			1639	1056	274	300	9			
1	G	209	Total	C	N	O	S	0	0	0
			1678	1085	279	305	9			
1	H	202	Total	C	N	O	S	0	0	0
			1627	1050	271	297	9			
1	J	209	Total	C	N	O	S	0	0	0
			1678	1085	279	305	9			
1	K	202	Total	C	N	O	S	0	0	0
			1627	1050	271	297	9			
1	M	201	Total	C	N	O	S	0	0	0
			1619	1046	270	294	9			
1	N	193	Total	C	N	O	S	0	0	0
			1557	1005	257	286	9			
1	P	200	Total	C	N	O	S	0	0	0
			1611	1040	269	293	9			
1	Q	196	Total	C	N	O	S	0	0	0
			1582	1023	261	289	9			
1	S	201	Total	C	N	O	S	0	0	0
			1615	1042	270	294	9			
1	T	192	Total	C	N	O	S	0	0	0
			1554	1005	256	284	9			
1	V	202	Total	C	N	O	S	0	0	0
			1627	1050	271	297	9			
1	W	192	Total	C	N	O	S	0	0	0
			1554	1005	256	284	9			

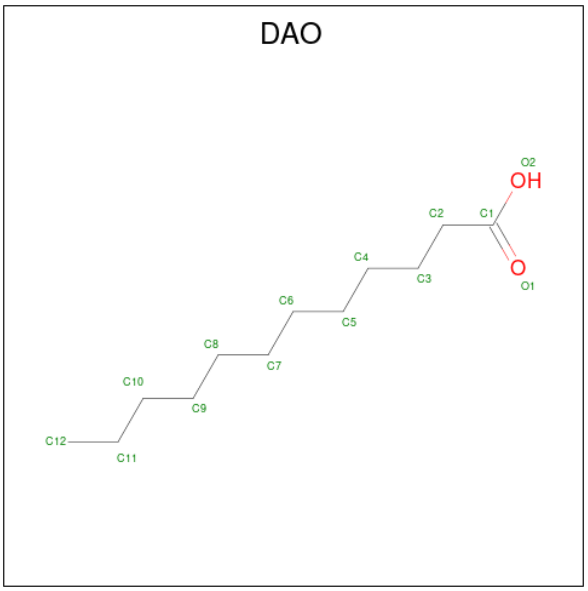
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLY	-	expression tag	UNP P41235
B	138	GLY	-	expression tag	UNP P41235
D	138	GLY	-	expression tag	UNP P41235
E	138	GLY	-	expression tag	UNP P41235
G	138	GLY	-	expression tag	UNP P41235
H	138	GLY	-	expression tag	UNP P41235
J	138	GLY	-	expression tag	UNP P41235
K	138	GLY	-	expression tag	UNP P41235
M	138	GLY	-	expression tag	UNP P41235
N	138	GLY	-	expression tag	UNP P41235
P	138	GLY	-	expression tag	UNP P41235
Q	138	GLY	-	expression tag	UNP P41235
S	138	GLY	-	expression tag	UNP P41235
T	138	GLY	-	expression tag	UNP P41235
V	138	GLY	-	expression tag	UNP P41235
W	138	GLY	-	expression tag	UNP P41235

- Molecule 2 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			52	35	8	9			
2	F	7	Total	C	N	O	0	0	0
			52	35	8	9			
2	I	7	Total	C	N	O	0	0	0
			52	35	8	9			
2	L	8	Total	C	N	O	0	0	0
			61	40	10	11			

- Molecule 3 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 12 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	D	1	Total C O 14 12 2	0	0
3	E	1	Total C O 14 12 2	0	0
3	G	1	Total C O 14 12 2	0	0
3	H	1	Total C O 14 12 2	0	0
3	J	1	Total C O 14 12 2	0	0
3	K	1	Total C O 14 12 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	6	Total O 6 6	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

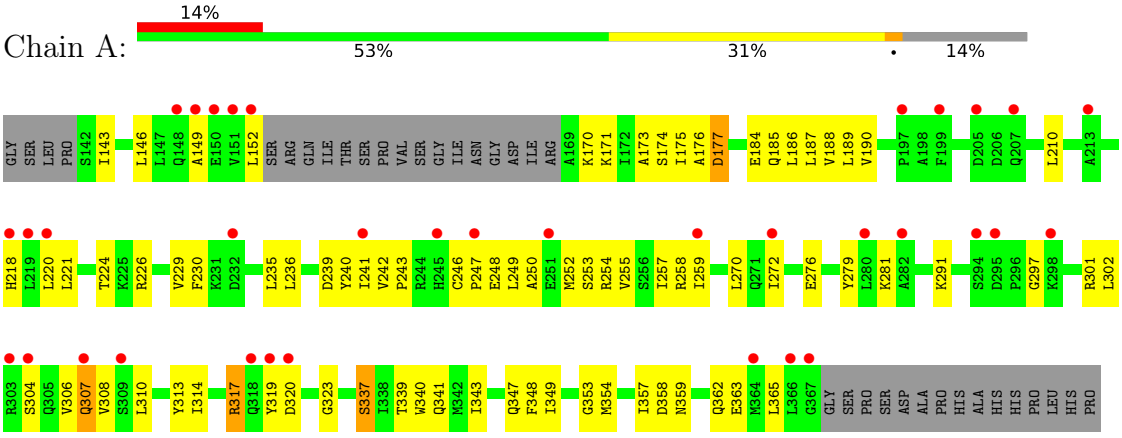
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total O 1 1	0	0
4	G	5	Total O 5 5	0	0
4	H	4	Total O 4 4	0	0
4	J	2	Total O 2 2	0	0
4	K	7	Total O 7 7	0	0
4	L	1	Total O 1 1	0	0
4	M	1	Total O 1 1	0	0
4	N	2	Total O 2 2	0	0
4	Q	1	Total O 1 1	0	0
4	S	2	Total O 2 2	0	0
4	V	2	Total O 2 2	0	0
4	W	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

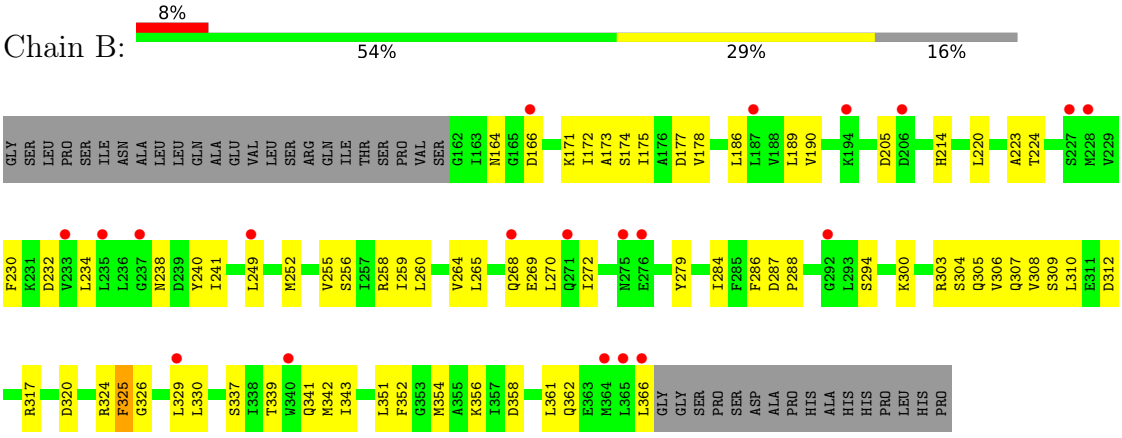
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain A:



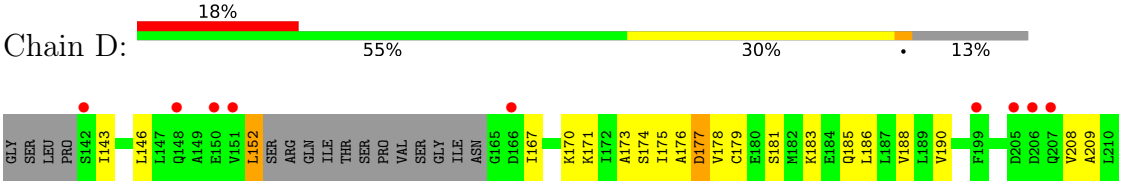
• Molecule 1: Hepatocyte nuclear factor 4-alpha

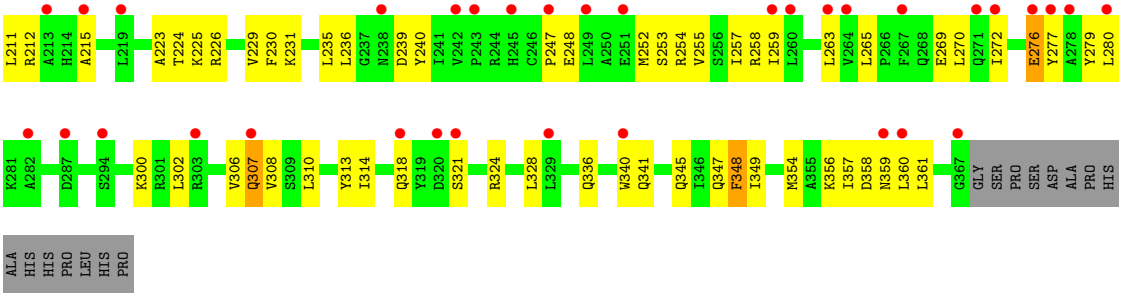
Chain B:



• Molecule 1: Hepatocyte nuclear factor 4-alpha

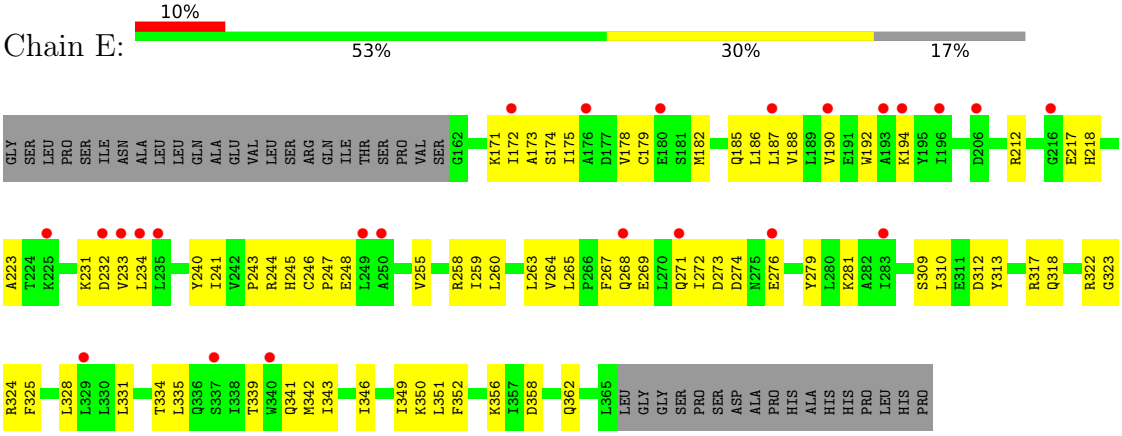
Chain D:





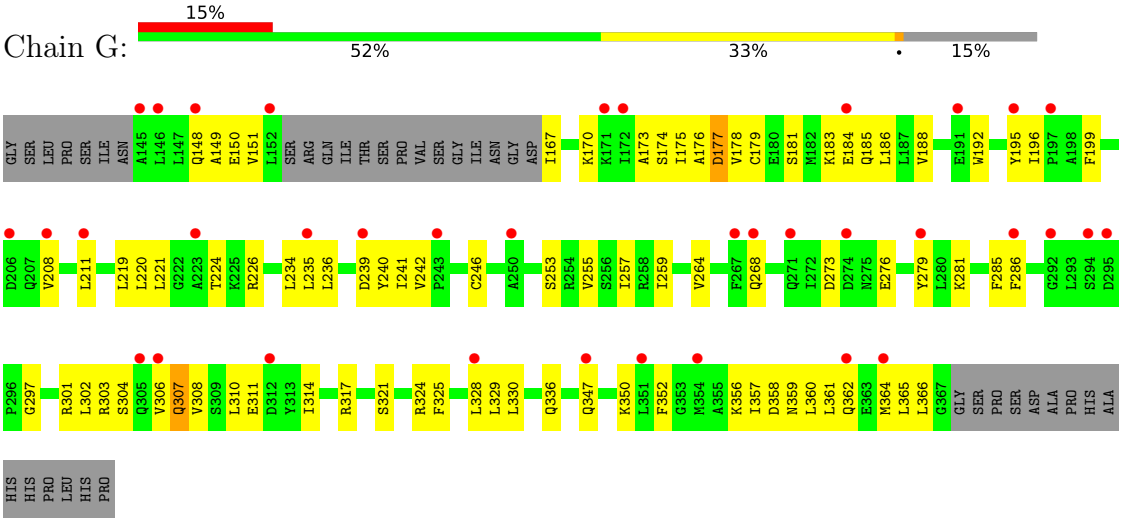
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain E:



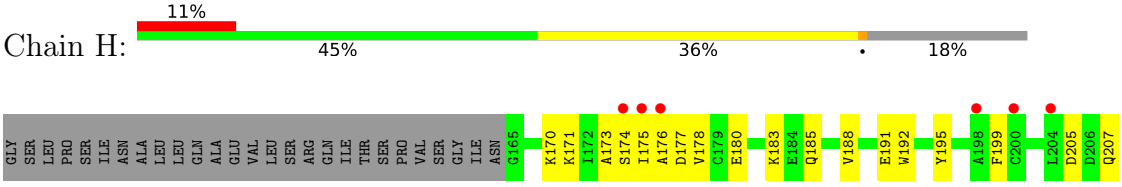
• Molecule 1: Hepatocyte nuclear factor 4-alpha

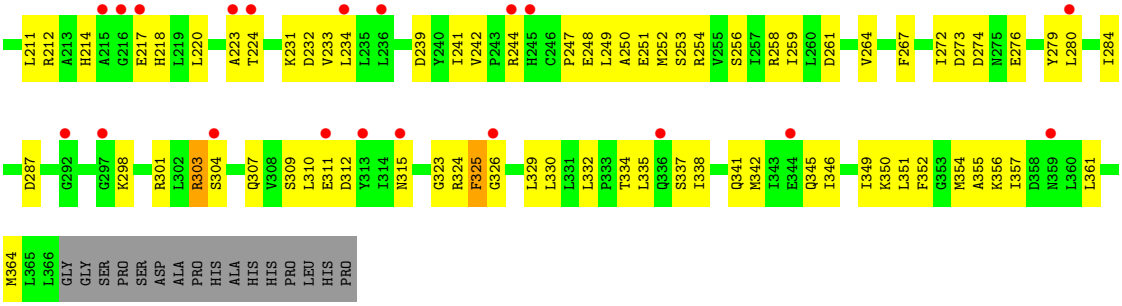
Chain G:



• Molecule 1: Hepatocyte nuclear factor 4-alpha

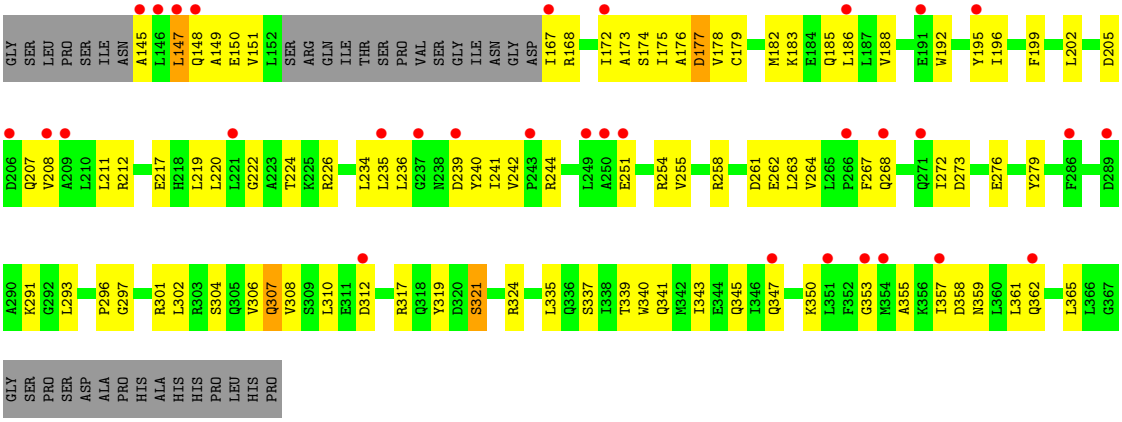
Chain H:





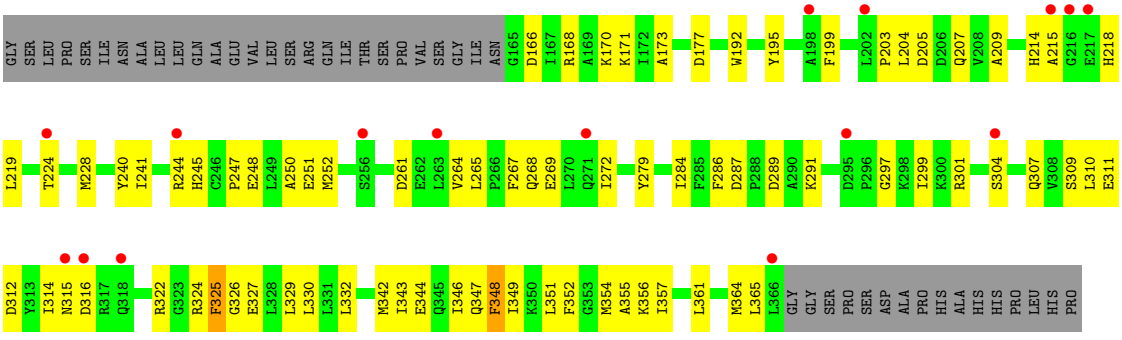
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain J:



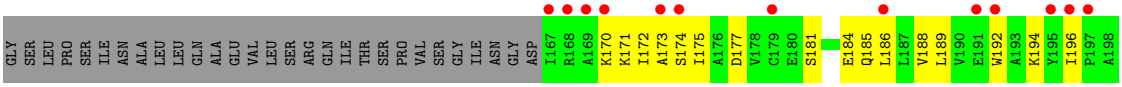
• Molecule 1: Hepatocyte nuclear factor 4-alpha

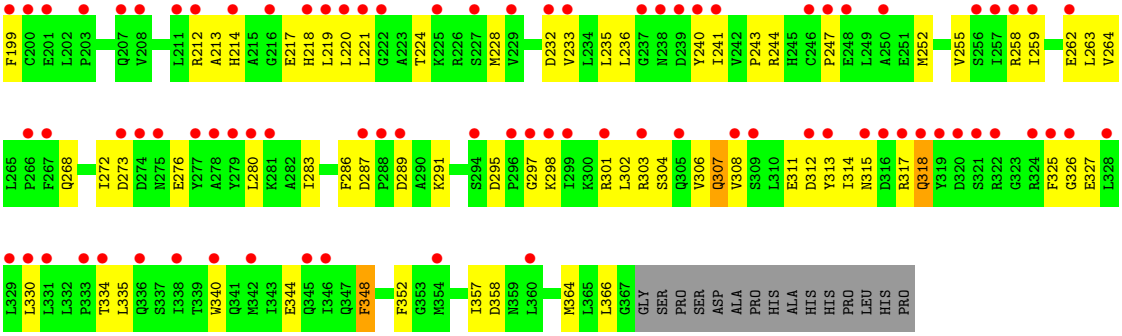
Chain K:



• Molecule 1: Hepatocyte nuclear factor 4-alpha

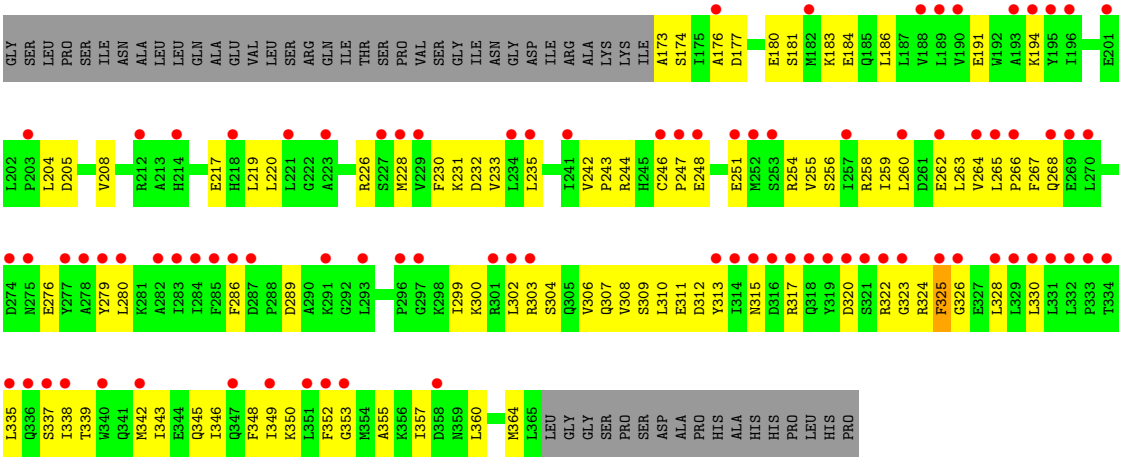
Chain M:





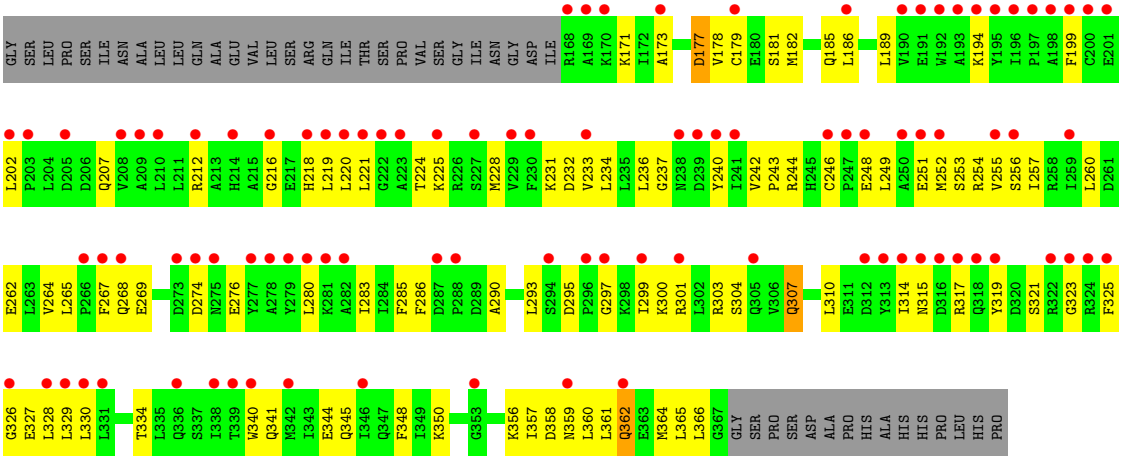
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain N:



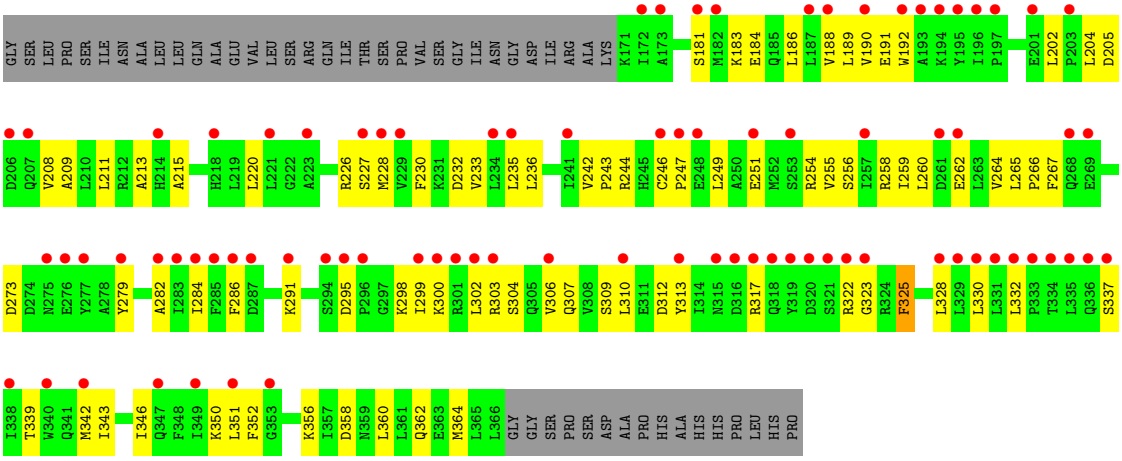
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain P:

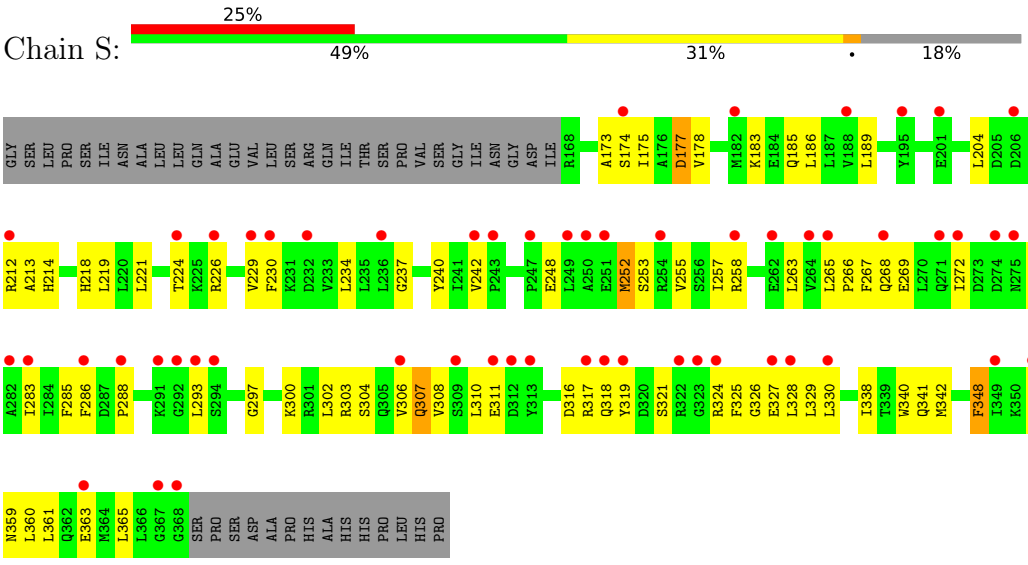


• Molecule 1: Hepatocyte nuclear factor 4-alpha

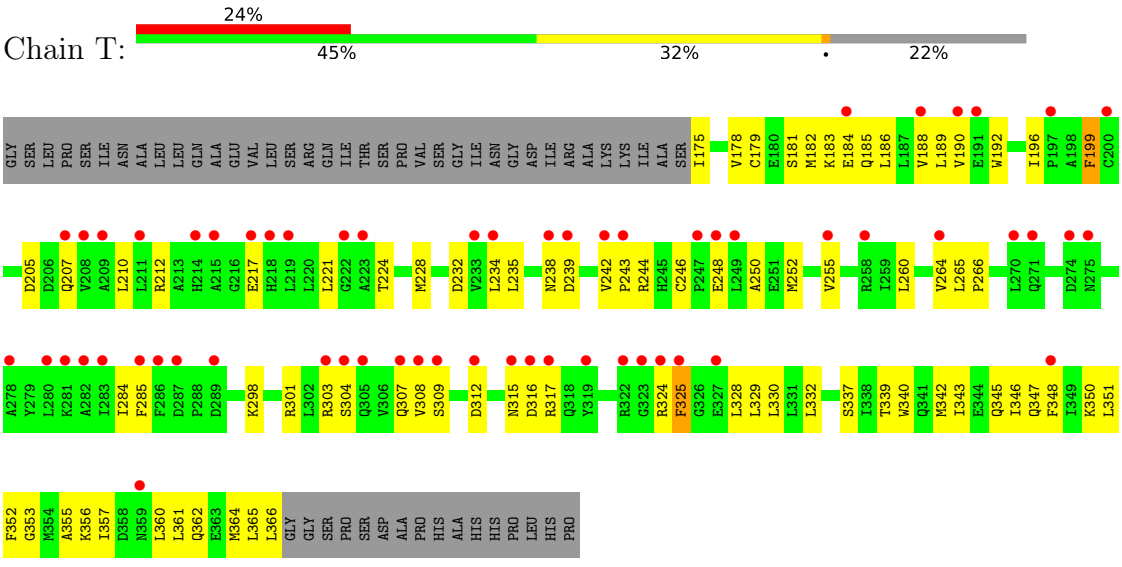
Chain Q:



• Molecule 1: Hepatocyte nuclear factor 4-alpha

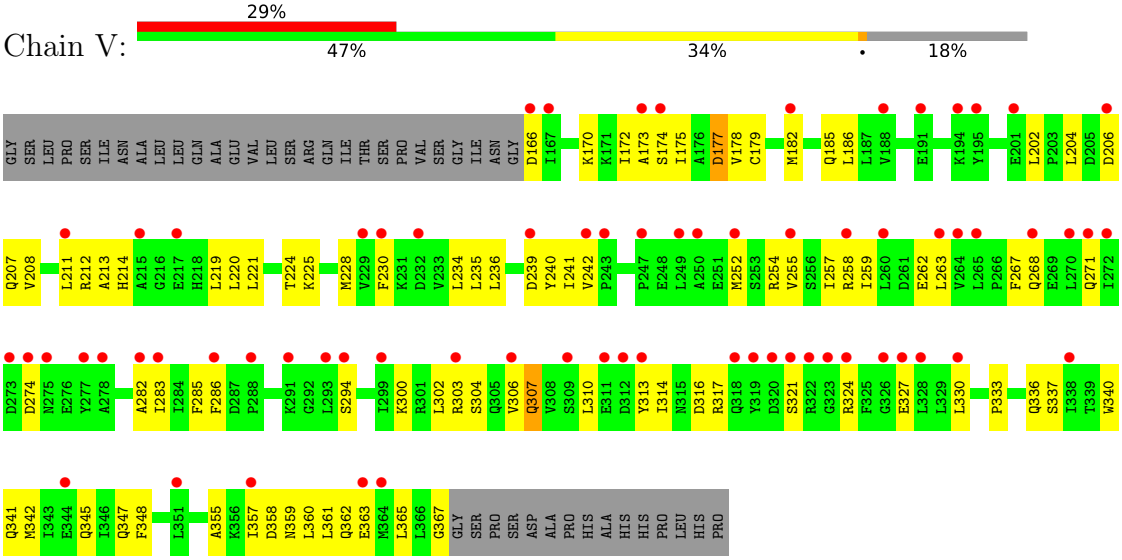


• Molecule 1: Hepatocyte nuclear factor 4-alpha



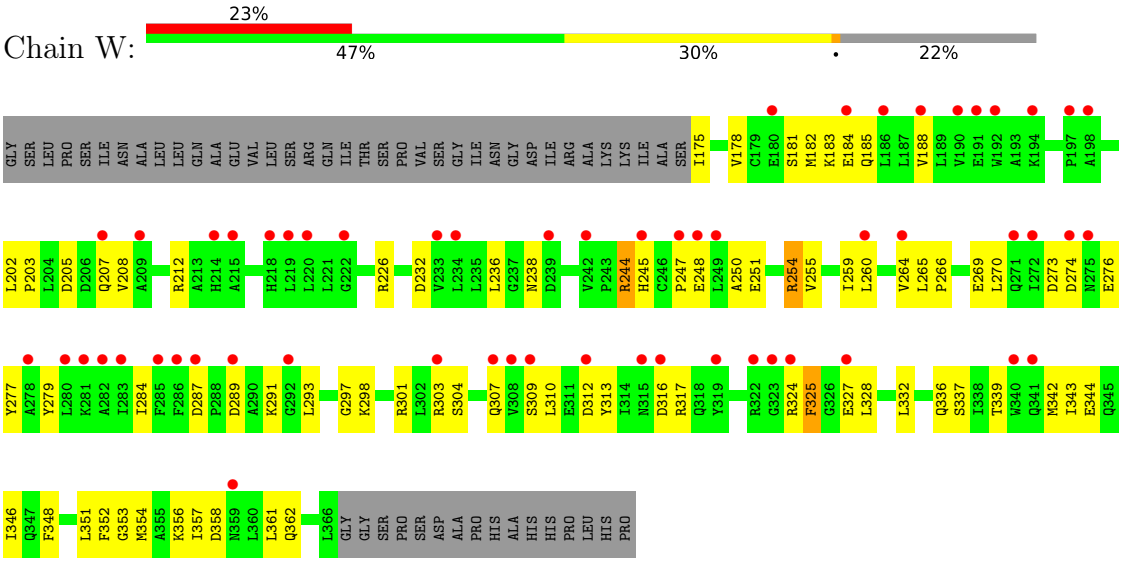
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain V:



• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain W:

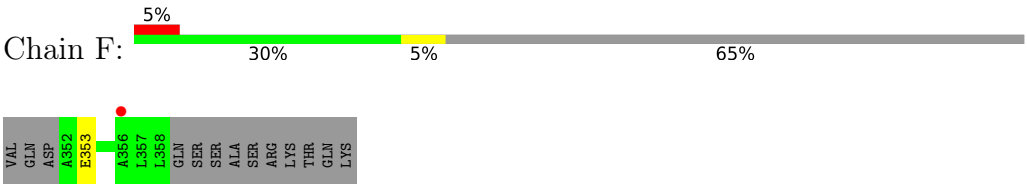


• Molecule 2: Proliferation-associated protein 2G4

Chain C:

• Molecule 2: Proliferation-associated protein 2G4

Chain F:

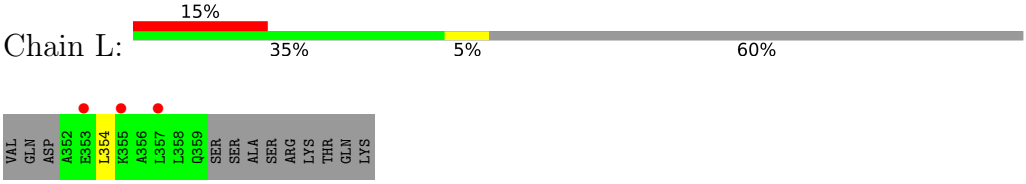


• Molecule 2: Proliferation-associated protein 2G4

Chain I:

• Molecule 2: Proliferation-associated protein 2G4

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	139.72Å 104.95Å 139.56Å 90.00° 90.61° 90.00°	Depositor
Resolution (Å)	49.63 – 3.17 49.63 – 3.17	Depositor EDS
% Data completeness (in resolution range)	71.6 (49.63-3.17) 71.6 (49.63-3.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	644.16 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.262 , 0.274 0.260 , 0.268	Depositor DCC
R_{free} test set	2505 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	66.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.046 for -l,k,h 0.056 for -h,-k,l 0.390 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26381	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5463e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.30	0/1708	0.52	0/2307
1	B	0.31	0/1675	0.54	0/2262
1	D	0.28	0/1739	0.50	0/2348
1	E	0.29	0/1667	0.52	0/2251
1	G	0.28	0/1705	0.52	0/2302
1	H	0.30	0/1655	0.53	0/2235
1	J	0.29	0/1705	0.53	0/2302
1	K	0.31	0/1655	0.55	0/2235
1	M	0.27	0/1647	0.51	0/2224
1	N	0.26	0/1585	0.47	0/2143
1	P	0.27	0/1639	0.50	0/2213
1	Q	0.27	0/1610	0.47	0/2176
1	S	0.28	0/1643	0.52	0/2218
1	T	0.28	0/1582	0.47	0/2139
1	V	0.29	0/1655	0.53	0/2235
1	W	0.28	0/1582	0.47	0/2139
2	C	0.26	0/51	0.45	0/67
2	F	0.24	0/51	0.48	0/67
2	I	0.24	0/51	0.67	0/67
2	L	0.24	0/60	0.65	0/79
All	All	0.28	0/26665	0.51	0/36009

There are no bond length outliers.

There are no bond angle outliers.

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	1681	0	1733	69	1
1	B	1647	0	1694	60	0
1	D	1712	0	1765	59	1
1	E	1639	0	1683	58	0
1	G	1678	0	1735	67	0
1	H	1627	0	1673	66	0
1	J	1678	0	1736	63	0
1	K	1627	0	1673	63	0
1	M	1619	0	1671	64	0
1	N	1557	0	1591	69	0
1	P	1611	0	1660	73	0
1	Q	1582	0	1626	70	0
1	S	1615	0	1663	61	0
1	T	1554	0	1592	66	1
1	V	1627	0	1675	69	0
1	W	1554	0	1592	68	1
2	C	52	0	61	3	0
2	F	52	0	61	1	0
2	I	52	0	61	4	0
2	L	61	0	69	2	0
3	A	14	0	23	1	0
3	B	14	0	23	2	0
3	D	14	0	23	3	0
3	E	14	0	23	2	0
3	G	14	0	23	3	0
3	H	14	0	23	2	0
3	J	14	0	23	2	0
3	K	14	0	23	1	0
4	A	6	0	0	0	0
4	B	6	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
4	G	5	0	0	0	0
4	H	4	0	0	0	0
4	J	2	0	0	0	0
4	K	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	2	0	0	0	0
4	Q	1	0	0	1	0
4	S	2	0	0	0	0
4	V	2	0	0	1	0
4	W	2	0	0	0	0
All	All	26381	0	27198	941	2

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 (941) 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:M:348:PHE:HE1	1:M:352:PHE:CE2	1.32	1.46
1:M:348:PHE:CE1	1:M:352:PHE:CE2	2.19	1.31
1:A:317:ARG:NE	1:A:319:TYR:CD2	2.25	1.04
1:A:317:ARG:CZ	1:A:319:TYR:CE2	2.51	0.93
1:A:317:ARG:CZ	1:A:319:TYR:CD2	2.53	0.91
1:M:348:PHE:CE1	1:M:352:PHE:HE2	1.78	0.90
1:A:317:ARG:NE	1:A:317:ARG:O	2.05	0.90
1:T:284:ILE:HD11	1:T:332:LEU:HD22	1.57	0.86
1:P:173:ALA:HB2	1:P:240:TYR:HB3	1.59	0.84
1:A:323:GLY:O	1:B:307:GLN:NE2	2.09	0.84
1:D:186:LEU:HD11	1:D:215:ALA:HB1	1.61	0.83
1:M:283:ILE:HG23	1:M:303:ARG:HD2	1.61	0.83
1:A:258:ARG:NH2	1:A:337:SER:OG	2.12	0.82
1:H:355:ALA:HB2	1:T:351:LEU:HD11	1.60	0.81
1:G:167:ILE:HA	1:G:170:LYS:HE2	1.59	0.81
1:A:323:GLY:HA3	1:B:308:VAL:HG22	1.63	0.80
1:P:260:LEU:HA	1:P:264:VAL:HG12	1.63	0.80
1:K:247:PRO:HA	1:K:250:ALA:HB2	1.62	0.80
1:Q:282:ALA:HB3	1:Q:306:VAL:HG11	1.62	0.80
1:W:358:ASP:O	1:W:362:GLN:NE2	2.15	0.79
1:W:284:ILE:HD11	1:W:332:LEU:HD22	1.63	0.79
1:V:230:PHE:O	1:V:268:GLN:NE2	2.15	0.79
1:B:249:LEU:HD21	1:B:252:MET:HB2	1.65	0.78
1:Q:243:PRO:HD2	1:Q:246:CYS:HB2	1.66	0.78
1:K:343:ILE:O	1:K:347:GLN:NE2	2.15	0.78
1:V:212:ARG:HH21	1:V:363:GLU:HG3	1.47	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:GLU:OE1	1:G:324:ARG:NH1	2.17	0.78
1:P:283:ILE:O	1:P:303:ARG:NH1	2.17	0.77
1:M:312:ASP:O	1:M:315:ASN:ND2	2.16	0.77
1:Q:286:PHE:HB3	1:Q:299:ILE:HG23	1.67	0.76
1:A:340:TRP:HH2	1:B:337:SER:HA	1.51	0.76
1:V:175:ILE:HD12	1:V:355:ALA:HB2	1.65	0.76
1:E:185:GLN:HA	1:E:188:VAL:HG12	1.66	0.76
1:V:170:LYS:HD3	1:V:239:ASP:HB3	1.66	0.76
1:A:258:ARG:NH1	1:A:341:GLN:OE1	2.19	0.76
1:E:212:ARG:HD2	1:H:183:LYS:HE2	1.67	0.75
1:T:304:SER:HA	1:T:307:GLN:HE21	1.50	0.75
1:M:348:PHE:HE1	1:M:352:PHE:CZ	2.00	0.75
1:B:189:LEU:O	1:B:189:LEU:HD23	1.86	0.74
1:E:260:LEU:HA	1:E:264:VAL:HB	1.68	0.74
1:G:352:PHE:HA	1:T:175:ILE:HD11	1.70	0.74
1:E:358:ASP:O	1:E:362:GLN:NE2	2.21	0.73
1:B:230:PHE:O	1:B:268:GLN:NE2	2.20	0.73
1:B:358:ASP:O	1:B:362:GLN:NE2	2.20	0.73
1:P:307:GLN:HE22	1:Q:330:LEU:HD11	1.52	0.73
1:K:214:HIS:ND1	1:K:284:ILE:O	2.19	0.73
1:D:209:ALA:HA	1:D:212:ARG:HE	1.55	0.72
1:V:340:TRP:HH2	1:W:337:SER:HA	1.54	0.72
1:M:224:THR:HG21	1:M:263:LEU:HD13	1.70	0.72
1:H:171:LYS:H	1:H:171:LYS:HD2	1.52	0.72
1:A:317:ARG:NH2	1:A:319:TYR:CE2	2.58	0.71
1:H:349:ILE:HG23	1:S:351:LEU:HD13	1.71	0.71
1:S:283:ILE:O	1:S:303:ARG:NH1	2.23	0.71
1:B:356:LYS:HZ1	1:M:348:PHE:HB2	1.54	0.71
1:D:347:GLN:NE2	1:Q:251:GLU:OE2	2.23	0.71
1:A:317:ARG:NH2	1:A:319:TYR:CZ	2.58	0.71
1:H:342:MET:O	1:H:346:ILE:HG13	1.91	0.71
1:H:311:GLU:HB2	1:H:325:PHE:HE2	1.55	0.70
1:H:354:MET:HE2	1:Q:358:ASP:HA	1.73	0.70
1:J:145:ALA:N	1:J:148:GLN:OE1	2.24	0.70
1:M:334:THR:OG1	1:N:289:ASP:OD1	2.10	0.70
1:W:232:ASP:HB3	1:W:244:ARG:HB2	1.73	0.70
1:J:208:VAL:HG23	2:L:354:LEU:HD22	1.72	0.70
1:H:276:GLU:OE2	1:H:324:ARG:NH2	2.22	0.70
1:T:361:LEU:O	1:T:365:LEU:HB2	1.92	0.70
1:V:283:ILE:O	1:V:303:ARG:NH1	2.25	0.70
1:V:340:TRP:CH2	1:W:337:SER:HA	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LYS:HE3	1:M:344:GLU:HG3	1.74	0.70
1:G:186:LEU:HD23	1:G:360:LEU:HG	1.71	0.70
1:T:260:LEU:HD23	1:T:264:VAL:HG21	1.73	0.70
1:A:347:GLN:NE2	1:N:251:GLU:OE2	2.24	0.70
1:H:350:LYS:HG3	1:H:354:MET:HE3	1.72	0.69
1:S:258:ARG:NH1	1:S:341:GLN:OE1	2.25	0.69
1:B:205:ASP:OD2	1:B:294:SER:OG	2.10	0.69
1:G:211:LEU:HD12	2:I:354:LEU:HD21	1.75	0.69
1:G:314:ILE:HG23	1:G:317:ARG:HD3	1.74	0.69
1:K:251:GLU:OE1	1:V:347:GLN:NE2	2.26	0.69
1:S:230:PHE:O	1:S:268:GLN:NE2	2.24	0.69
1:E:273:ASP:HB2	1:E:317:ARG:HH12	1.58	0.69
1:E:273:ASP:OD2	1:E:313:TYR:OH	2.10	0.68
1:P:212:ARG:NH2	1:P:366:LEU:O	2.26	0.68
1:Q:284:ILE:HD11	1:Q:332:LEU:HB3	1.75	0.68
1:D:258:ARG:NH1	1:D:341:GLN:OE1	2.26	0.68
1:M:185:GLN:HB3	1:M:219:LEU:HD22	1.74	0.68
1:Q:342:MET:O	1:Q:346:ILE:HG13	1.93	0.68
1:H:249:LEU:O	1:H:253:SER:N	2.26	0.68
1:K:279:TYR:HD2	1:K:310:LEU:HD23	1.58	0.68
1:S:185:GLN:HB3	1:S:219:LEU:HD22	1.74	0.67
1:N:300:LYS:HZ2	1:N:303:ARG:HE	1.43	0.67
1:K:355:ALA:HB2	1:W:351:LEU:HD11	1.75	0.67
1:N:208:VAL:HG13	1:W:183:LYS:HG2	1.76	0.67
1:S:340:TRP:CH2	1:T:337:SER:HA	2.30	0.66
1:H:258:ARG:NH1	1:H:341:GLN:OE1	2.28	0.66
1:G:148:GLN:NE2	1:G:195:TYR:O	2.29	0.66
1:M:304:SER:O	1:M:308:VAL:HG23	1.95	0.66
1:V:212:ARG:NH2	4:V:700:HOH:O	2.28	0.66
1:V:283:ILE:HA	1:V:303:ARG:HD2	1.76	0.66
1:V:327:GLU:OE2	1:W:303:ARG:NH2	2.28	0.66
1:K:342:MET:O	1:K:346:ILE:HG13	1.94	0.66
1:B:171:LYS:NZ	1:B:172:ILE:O	2.26	0.66
1:M:212:ARG:NH2	1:M:366:LEU:O	2.27	0.66
1:J:211:LEU:HD12	2:L:354:LEU:HD21	1.78	0.66
1:S:183:LYS:HG3	1:S:360:LEU:HD22	1.77	0.65
1:K:344:GLU:O	1:K:348:PHE:HB2	1.96	0.65
1:W:298:LYS:HG3	1:W:301:ARG:HH21	1.62	0.65
1:G:286:PHE:O	1:G:303:ARG:HD3	1.97	0.65
1:V:304:SER:OG	1:W:327:GLU:OE2	2.11	0.65
1:E:271:GLN:O	1:E:324:ARG:NH2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:LEU:HD13	1:M:241:ILE:HG22	1.80	0.64
1:V:173:ALA:HB2	1:V:240:TYR:HB3	1.79	0.64
1:V:316:ASP:HA	1:V:321:SER:HB3	1.80	0.64
1:A:149:ALA:HA	1:A:152:LEU:HD13	1.79	0.64
1:Q:227:SER:HB3	1:Q:235:LEU:H	1.62	0.64
1:Q:258:ARG:NH2	1:Q:262:GLU:OE2	2.31	0.64
1:Q:358:ASP:O	1:Q:362:GLN:NE2	2.29	0.63
1:Q:220:LEU:HD21	1:Q:342:MET:HE1	1.80	0.63
1:T:342:MET:O	1:T:346:ILE:HG13	1.98	0.63
1:M:276:GLU:OE2	1:M:317:ARG:NH2	2.31	0.63
1:S:304:SER:O	1:S:308:VAL:HG23	1.99	0.63
1:T:199:PHE:O	1:T:207:GLN:NE2	2.31	0.63
1:J:317:ARG:HB3	1:J:321:SER:OG	1.98	0.63
1:H:279:TYR:HD2	1:H:310:LEU:HD23	1.63	0.63
1:W:260:LEU:HD23	1:W:264:VAL:HG21	1.80	0.63
1:D:235:LEU:HD11	1:D:239:ASP:HA	1.80	0.63
1:B:317:ARG:NH1	1:B:320:ASP:O	2.31	0.63
1:A:363:GLU:OE2	2:C:352:ALA:N	2.32	0.62
1:G:304:SER:O	1:G:308:VAL:HG23	1.99	0.62
1:J:186:LEU:HD22	1:J:361:LEU:HD12	1.81	0.62
1:Q:202:LEU:HD21	1:Q:298:LYS:HE3	1.81	0.62
1:M:287:ASP:OD1	1:M:303:ARG:NH1	2.33	0.62
1:T:298:LYS:HG3	1:T:301:ARG:HH22	1.65	0.62
1:E:259:ILE:HG22	1:E:264:VAL:HG23	1.80	0.62
1:P:225:LYS:NZ	1:P:274:ASP:OD1	2.23	0.62
1:B:260:LEU:HA	1:B:264:VAL:HB	1.81	0.62
1:E:175:ILE:HD12	1:T:365:LEU:HD23	1.81	0.62
1:E:342:MET:O	1:E:346:ILE:HG13	1.98	0.62
1:G:149:ALA:HB1	1:G:192:TRP:O	1.99	0.62
1:D:174:SER:OG	1:D:177:ASP:OD1	2.14	0.62
1:D:186:LEU:HD23	1:D:360:LEU:HG	1.80	0.62
1:K:286:PHE:HB3	1:K:299:ILE:HG23	1.82	0.62
1:S:340:TRP:HH2	1:T:337:SER:HA	1.64	0.62
1:A:220:LEU:O	1:A:224:THR:HG23	1.98	0.62
1:H:199:PHE:O	1:H:207:GLN:NE2	2.32	0.62
1:P:202:LEU:O	1:P:207:GLN:NE2	2.32	0.62
1:P:360:LEU:O	1:P:364:MET:HB2	2.00	0.62
1:V:225:LYS:NZ	1:V:274:ASP:OD1	2.32	0.62
1:M:273:ASP:OD2	1:M:317:ARG:NH2	2.27	0.62
1:P:356:LYS:H	1:P:356:LYS:HD2	1.64	0.62
1:S:327:GLU:OE1	1:T:307:GLN:NE2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HD21	1:N:355:ALA:HB2	1.81	0.61
1:J:312:ASP:OD2	1:K:322:ARG:NH2	2.33	0.61
1:D:358:ASP:OD1	1:D:359:ASN:N	2.32	0.61
1:W:276:GLU:OE2	1:W:317:ARG:NH1	2.33	0.61
1:N:317:ARG:NH1	1:N:320:ASP:O	2.33	0.61
1:P:327:GLU:OE2	1:Q:307:GLN:HG2	2.00	0.61
1:B:356:LYS:NZ	1:M:348:PHE:HB2	2.15	0.61
1:H:224:THR:HG23	1:H:264:VAL:HG22	1.82	0.61
1:J:304:SER:O	1:J:308:VAL:HG23	2.01	0.61
1:Q:232:ASP:HB3	1:Q:244:ARG:HB2	1.81	0.61
1:V:234:LEU:O	1:V:242:VAL:N	2.31	0.61
1:J:202:LEU:O	1:J:207:GLN:NE2	2.34	0.61
1:K:279:TYR:CD2	1:K:310:LEU:HD23	2.34	0.61
1:M:327:GLU:HA	1:M:330:LEU:HD12	1.81	0.61
1:P:357:ILE:HG22	1:P:358:ASP:H	1.66	0.61
1:A:173:ALA:HB2	1:A:240:TYR:HB3	1.83	0.61
1:V:255:VAL:HG11	1:V:342:MET:HB2	1.82	0.61
1:E:258:ARG:NH1	1:E:341:GLN:OE1	2.33	0.60
1:G:181:SER:OG	3:G:500:DAO:O1	2.19	0.60
1:S:304:SER:O	1:S:307:GLN:HG2	2.01	0.60
1:S:358:ASP:OD1	1:S:359:ASN:N	2.34	0.60
1:H:357:ILE:HD11	1:S:348:PHE:HZ	1.66	0.60
1:A:317:ARG:CZ	1:A:317:ARG:O	2.49	0.60
1:D:349:ILE:HG23	1:D:354:MET:HB2	1.82	0.60
1:A:249:LEU:HB3	1:A:252:MET:HB2	1.83	0.60
1:T:347:GLN:HA	1:T:350:LYS:HE2	1.84	0.60
1:W:358:ASP:OD1	1:W:362:GLN:NE2	2.35	0.60
1:B:189:LEU:HD23	1:B:189:LEU:C	2.21	0.60
1:J:185:GLN:HB3	1:J:219:LEU:HD22	1.82	0.60
1:K:214:HIS:O	1:K:218:HIS:ND1	2.33	0.60
1:K:314:ILE:HD12	1:K:324:ARG:HG2	1.82	0.60
1:Q:339:THR:O	1:Q:343:ILE:HG13	2.02	0.60
1:D:152:LEU:HD23	1:D:152:LEU:H	1.66	0.60
1:B:259:ILE:HG22	1:B:264:VAL:HG23	1.84	0.59
1:B:214:HIS:ND1	1:B:284:ILE:O	2.28	0.59
1:S:173:ALA:HB2	1:S:240:TYR:HB3	1.84	0.59
1:V:337:SER:HB3	1:W:336:GLN:NE2	2.17	0.59
1:H:326:GLY:O	1:H:330:LEU:HG	2.03	0.59
1:J:234:LEU:O	1:J:242:VAL:N	2.31	0.59
1:J:343:ILE:HG12	1:J:365:LEU:HD23	1.84	0.59
1:V:185:GLN:HE21	1:V:219:LEU:HD22	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:GLN:HG3	3:G:500:DAO:H32	1.83	0.59
1:G:297:GLY:O	1:G:301:ARG:HG3	2.03	0.59
1:W:353:GLY:O	1:W:357:ILE:HG13	2.03	0.59
1:N:208:VAL:CG1	1:W:183:LYS:HG2	2.32	0.59
1:W:276:GLU:OE1	1:W:324:ARG:NH2	2.36	0.59
1:J:220:LEU:O	1:J:224:THR:HG23	2.02	0.58
1:V:202:LEU:O	1:V:207:GLN:NE2	2.36	0.58
1:A:242:VAL:HG13	1:A:246:CYS:SG	2.43	0.58
1:J:276:GLU:OE2	1:J:324:ARG:NH1	2.35	0.58
1:J:173:ALA:HB1	1:J:177:ASP:HB2	1.84	0.58
1:J:264:VAL:O	1:J:268:GLN:HG3	2.04	0.58
1:P:260:LEU:HD23	1:P:264:VAL:HG11	1.85	0.58
1:Q:273:ASP:OD2	1:Q:317:ARG:NH1	2.36	0.58
1:W:339:THR:O	1:W:343:ILE:HG13	2.03	0.58
1:B:351:LEU:HD13	1:N:352:PHE:HA	1.85	0.58
1:P:234:LEU:O	1:P:242:VAL:N	2.29	0.58
1:N:232:ASP:HB3	1:N:244:ARG:HB2	1.85	0.58
1:W:226:ARG:HH21	1:W:236:LEU:HA	1.68	0.58
1:W:208:VAL:HG13	1:W:212:ARG:CZ	2.32	0.58
1:H:280:LEU:HD21	1:H:332:LEU:HD21	1.86	0.58
1:K:215:ALA:O	1:K:219:LEU:HD22	2.04	0.58
1:H:352:PHE:CZ	1:H:356:LYS:HD3	2.38	0.58
1:S:357:ILE:HG22	1:S:358:ASP:H	1.68	0.58
1:B:325:PHE:HE1	1:B:329:LEU:HD11	1.69	0.57
1:E:218:HIS:NE2	1:E:281:LYS:HG3	2.19	0.57
1:G:317:ARG:HB3	1:G:321:SER:HB3	1.86	0.57
1:J:276:GLU:CD	1:J:324:ARG:HH12	2.07	0.57
1:P:262:GLU:HB3	1:P:334:THR:HG21	1.86	0.57
1:S:173:ALA:HB1	1:S:177:ASP:HB2	1.85	0.57
1:G:208:VAL:HG22	2:I:354:LEU:HD22	1.85	0.57
1:P:260:LEU:HA	1:P:264:VAL:CG1	2.34	0.57
1:S:317:ARG:O	1:S:317:ARG:HD3	2.03	0.57
1:D:143:ILE:HD12	1:D:146:LEU:HD12	1.86	0.57
1:E:171:LYS:NZ	1:E:172:ILE:O	2.30	0.57
1:Q:242:VAL:HG13	1:Q:249:LEU:HD21	1.86	0.57
1:W:266:PRO:HA	1:W:269:GLU:HG2	1.85	0.57
1:K:166:ASP:O	1:K:168:ARG:NE	2.38	0.57
1:P:173:ALA:HB1	1:P:177:ASP:HB2	1.86	0.57
1:V:224:THR:HG1	1:V:267:PHE:HE2	1.52	0.57
1:K:214:HIS:CE1	1:K:287:ASP:HB2	2.38	0.57
1:A:173:ALA:HA	1:A:240:TYR:HD2	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:VAL:HG21	2:I:355:LYS:HG2	1.86	0.57
1:K:252:MET:HE1	1:K:349:ILE:HD12	1.87	0.57
1:S:327:GLU:OE2	1:T:303:ARG:NH2	2.37	0.57
1:D:190:VAL:HG22	1:D:211:LEU:HD13	1.87	0.56
1:G:183:LYS:HG2	1:G:361:LEU:HD13	1.87	0.56
1:H:251:GLU:O	1:H:345:GLN:NE2	2.38	0.56
1:V:304:SER:O	1:V:307:GLN:HG2	2.05	0.56
1:V:327:GLU:HA	1:V:330:LEU:HD12	1.87	0.56
1:N:226:ARG:HG2	1:N:235:LEU:HD23	1.86	0.56
1:B:304:SER:O	1:B:308:VAL:HG23	2.06	0.56
1:B:258:ARG:NH1	1:B:341:GLN:OE1	2.39	0.56
1:N:339:THR:O	1:N:343:ILE:HG13	2.06	0.56
1:S:255:VAL:HG11	1:S:342:MET:HB2	1.86	0.56
1:W:202:LEU:O	1:W:207:GLN:NE2	2.38	0.56
1:D:183:LYS:HG2	1:D:361:LEU:HD13	1.88	0.56
1:K:252:MET:HG2	3:K:500:DAO:H121	1.86	0.56
1:D:336:GLN:HG2	1:D:340:TRP:CD1	2.41	0.56
1:E:248:GLU:O	1:P:350:LYS:NZ	2.39	0.56
1:J:186:LEU:HD12	1:J:219:LEU:HD21	1.86	0.56
1:B:252:MET:HB3	3:B:500:DAO:H121	1.86	0.56
1:D:314:ILE:HG21	1:D:324:ARG:HB3	1.88	0.56
1:K:357:ILE:HD11	1:V:348:PHE:HZ	1.71	0.56
1:M:330:LEU:HD13	1:N:303:ARG:NH2	2.21	0.56
1:T:186:LEU:HD12	1:T:189:LEU:HD12	1.87	0.56
1:W:342:MET:O	1:W:346:ILE:HG13	2.05	0.56
1:M:173:ALA:HB2	1:M:240:TYR:O	2.06	0.55
1:N:220:LEU:HD21	1:N:342:MET:HE1	1.88	0.55
1:N:325:PHE:HA	1:N:328:LEU:HD12	1.87	0.55
1:Q:209:ALA:HB1	1:Q:291:LYS:O	2.06	0.55
1:V:336:GLN:NE2	1:W:336:GLN:OE1	2.38	0.55
1:D:185:GLN:HA	1:D:188:VAL:HG22	1.88	0.55
1:E:178:VAL:O	1:E:182:MET:HG3	2.06	0.55
1:P:304:SER:O	1:P:307:GLN:HG2	2.06	0.55
1:A:340:TRP:CH2	1:B:337:SER:HA	2.39	0.55
1:E:279:TYR:CD2	1:E:310:LEU:HA	2.42	0.55
1:G:150:GLU:N	1:G:192:TRP:HD1	2.05	0.55
1:V:271:GLN:O	1:V:324:ARG:NH2	2.40	0.55
1:J:234:LEU:HB2	1:J:242:VAL:HB	1.88	0.55
1:S:327:GLU:HB2	1:T:307:GLN:HE22	1.71	0.55
1:G:246:CYS:HB2	1:G:253:SER:HB3	1.87	0.55
1:M:228:MET:O	1:M:268:GLN:HG2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:SER:O	1:D:257:ILE:HG13	2.07	0.55
1:N:259:ILE:HG12	1:N:338:ILE:HD13	1.89	0.55
1:Q:304:SER:O	1:Q:307:GLN:HG3	2.07	0.55
1:G:150:GLU:OE1	1:G:281:LYS:NZ	2.40	0.55
1:P:251:GLU:OE1	1:P:254:ARG:NH1	2.37	0.55
1:S:173:ALA:HB2	1:S:240:TYR:CG	2.41	0.55
1:D:356:LYS:H	1:D:356:LYS:HD3	1.72	0.55
1:H:174:SER:O	1:H:178:VAL:HG23	2.07	0.55
1:Q:309:SER:HA	1:Q:312:ASP:OD2	2.07	0.55
1:V:173:ALA:HB1	1:V:177:ASP:HB2	1.89	0.55
1:B:256:SER:HA	1:B:259:ILE:HD12	1.89	0.54
1:H:334:THR:O	1:H:338:ILE:HG12	2.07	0.54
1:J:235:LEU:HD11	1:J:239:ASP:HA	1.89	0.54
1:T:360:LEU:O	1:T:364:MET:HG2	2.07	0.54
1:A:173:ALA:HA	1:A:240:TYR:CD2	2.42	0.54
1:H:217:GLU:HA	1:H:335:LEU:HD11	1.88	0.54
1:P:220:LEU:O	1:P:224:THR:HG23	2.08	0.54
1:V:357:ILE:HG22	1:V:358:ASP:H	1.72	0.54
1:H:279:TYR:CD2	1:H:310:LEU:HD23	2.43	0.54
1:M:276:GLU:O	1:M:280:LEU:HB2	2.08	0.54
1:V:333:PRO:O	1:W:336:GLN:NE2	2.35	0.54
1:J:335:LEU:O	1:J:339:THR:OG1	2.22	0.54
1:M:303:ARG:HE	1:N:330:LEU:HD13	1.71	0.54
1:T:232:ASP:CG	1:T:244:ARG:HD3	2.28	0.54
1:A:358:ASP:OD1	1:A:359:ASN:N	2.41	0.54
1:B:175:ILE:O	1:B:178:VAL:HG22	2.07	0.54
1:B:272:ILE:HA	1:B:324:ARG:HH22	1.71	0.54
1:E:273:ASP:OD1	1:E:274:ASP:N	2.40	0.54
1:K:352:PHE:CZ	1:K:356:LYS:HD2	2.42	0.54
1:S:283:ILE:HA	1:S:303:ARG:HD2	1.89	0.54
1:G:329:LEU:HD12	1:H:329:LEU:HD12	1.89	0.54
1:G:234:LEU:O	1:G:242:VAL:N	2.39	0.54
1:K:173:ALA:HB1	1:K:177:ASP:HB2	1.90	0.54
1:M:220:LEU:O	1:M:224:THR:HG23	2.07	0.54
1:V:212:ARG:NE	1:V:363:GLU:O	2.39	0.54
1:N:183:LYS:HB3	1:W:212:ARG:NH2	2.23	0.54
1:W:208:VAL:HG13	1:W:212:ARG:NH2	2.23	0.54
1:A:320:ASP:OD1	1:A:320:ASP:N	2.41	0.54
1:D:226:ARG:NH2	1:D:235:LEU:O	2.35	0.54
1:D:231:LYS:HD3	1:K:268:GLN:NE2	2.23	0.54
1:K:364:MET:HB3	1:V:254:ARG:HH22	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:O	1:A:353:GLY:N	2.41	0.54
1:H:273:ASP:OD1	1:H:274:ASP:N	2.38	0.54
1:J:251:GLU:OE1	1:J:254:ARG:NH1	2.39	0.54
1:K:205:ASP:N	1:K:205:ASP:OD1	2.40	0.54
1:M:295:ASP:OD2	1:M:298:LYS:NZ	2.40	0.54
1:V:220:LEU:O	1:V:224:THR:HG23	2.08	0.54
1:B:224:THR:HG23	1:B:264:VAL:HG22	1.91	0.53
1:P:327:GLU:OE1	1:Q:307:GLN:NE2	2.42	0.53
1:Q:226:ARG:HH21	1:Q:236:LEU:HA	1.73	0.53
1:D:186:LEU:HB3	1:D:360:LEU:HD21	1.90	0.53
1:G:226:ARG:HH21	1:G:236:LEU:HA	1.73	0.53
1:M:172:ILE:HD13	1:M:247:PRO:HD2	1.89	0.53
1:M:286:PHE:O	1:M:303:ARG:HD3	2.09	0.53
1:P:249:LEU:HB2	1:P:253:SER:HB3	1.91	0.53
1:P:326:GLY:O	1:P:330:LEU:HG	2.07	0.53
1:M:217:GLU:HB3	1:M:335:LEU:HD21	1.89	0.53
1:N:183:LYS:HB3	1:W:212:ARG:CZ	2.38	0.53
1:Q:279:TYR:HB3	1:Q:310:LEU:HB2	1.91	0.53
1:S:212:ARG:NE	1:S:363:GLU:O	2.41	0.53
1:W:279:TYR:HD2	1:W:310:LEU:HD23	1.73	0.53
1:G:186:LEU:HD13	1:G:219:LEU:HD11	1.91	0.53
1:P:182:MET:HA	1:P:185:GLN:HG2	1.90	0.53
1:B:249:LEU:HG	1:B:252:MET:H	1.73	0.53
1:E:185:GLN:O	1:E:188:VAL:HG12	2.08	0.53
1:E:247:PRO:O	1:P:362:GLN:NE2	2.42	0.53
1:N:256:SER:HA	1:N:259:ILE:HD12	1.89	0.53
1:A:235:LEU:HD11	1:A:239:ASP:HA	1.88	0.53
1:B:309:SER:HA	1:B:312:ASP:OD2	2.08	0.53
1:D:272:ILE:HG23	1:D:276:GLU:HB2	1.91	0.53
1:S:325:PHE:CZ	1:S:329:LEU:HD11	2.44	0.53
1:W:269:GLU:HG3	1:W:270:LEU:HG	1.89	0.53
1:M:214:HIS:HB3	1:M:217:GLU:HB2	1.91	0.53
1:P:303:ARG:HE	1:Q:330:LEU:HD13	1.73	0.53
1:P:310:LEU:HD12	1:P:325:PHE:CE1	2.44	0.53
1:M:174:SER:OG	1:M:175:ILE:N	2.42	0.53
1:B:220:LEU:HD21	1:B:342:MET:HE1	1.90	0.53
1:E:179:CYS:SG	1:T:366:LEU:HD22	2.48	0.53
1:J:179:CYS:O	1:J:183:LYS:HG3	2.09	0.52
1:H:244:ARG:NH1	1:H:261:ASP:OD1	2.37	0.52
1:N:217:GLU:HB3	1:N:335:LEU:HD21	1.90	0.52
1:W:251:GLU:O	1:W:254:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:286:PHE:HB2	1:N:303:ARG:HD3	1.92	0.52
1:T:234:LEU:HB2	1:T:242:VAL:HB	1.91	0.52
1:B:352:PHE:CZ	1:B:356:LYS:HD2	2.44	0.52
1:E:339:THR:O	1:E:343:ILE:HG13	2.09	0.52
1:K:203:PRO:HB2	1:K:205:ASP:OD1	2.10	0.52
1:V:212:ARG:HD3	1:V:367:GLY:HA2	1.91	0.52
1:Q:279:TYR:HE2	1:Q:313:TYR:HB2	1.74	0.52
1:W:298:LYS:HA	1:W:301:ARG:HE	1.74	0.52
1:A:253:SER:O	1:A:257:ILE:HG12	2.10	0.52
1:E:351:LEU:HD13	1:Q:352:PHE:HA	1.92	0.52
1:V:224:THR:O	1:V:228:MET:HB3	2.10	0.52
1:P:232:ASP:HB3	1:P:244:ARG:HB2	1.90	0.52
1:D:357:ILE:HG22	1:D:358:ASP:H	1.74	0.52
1:K:357:ILE:O	1:K:361:LEU:HG	2.10	0.52
1:V:358:ASP:OD1	1:V:359:ASN:N	2.43	0.52
1:M:189:LEU:HD21	1:M:218:HIS:CD2	2.44	0.52
1:E:218:HIS:CE1	1:E:281:LYS:HG3	2.45	0.51
1:A:302:LEU:O	1:A:306:VAL:HG23	2.10	0.51
1:G:357:ILE:HG22	1:G:358:ASP:H	1.76	0.51
1:N:300:LYS:HZ3	1:N:303:ARG:HH21	1.57	0.51
1:P:315:ASN:HA	1:P:321:SER:OG	2.11	0.51
1:G:307:GLN:NE2	1:H:323:GLY:HA2	2.25	0.51
1:H:280:LEU:O	1:H:284:ILE:HG22	2.09	0.51
1:N:191:GLU:HA	1:N:194:LYS:HB2	1.93	0.51
1:P:358:ASP:OD1	1:P:359:ASN:N	2.43	0.51
1:T:352:PHE:CZ	1:T:356:LYS:HD2	2.46	0.51
1:V:236:LEU:HB2	1:V:240:TYR:HB2	1.92	0.51
1:A:317:ARG:NH2	1:A:319:TYR:CE1	2.79	0.51
1:A:349:ILE:HG23	1:A:354:MET:HB2	1.93	0.51
1:E:185:GLN:CA	1:E:188:VAL:HG12	2.37	0.51
1:Q:360:LEU:O	1:Q:364:MET:HG2	2.11	0.51
1:D:208:VAL:O	1:D:212:ARG:HG2	2.10	0.51
1:G:236:LEU:HD22	3:G:500:DAO:H22	1.90	0.51
1:M:326:GLY:O	1:M:330:LEU:HG	2.10	0.51
1:V:211:LEU:HD23	1:V:285:PHE:HE1	1.76	0.51
1:J:236:LEU:HB2	1:J:240:TYR:HB2	1.93	0.51
1:J:273:ASP:N	1:J:276:GLU:OE1	2.41	0.51
1:G:302:LEU:O	1:G:306:VAL:HG23	2.11	0.50
1:M:348:PHE:CE1	1:M:352:PHE:CD2	2.94	0.50
1:P:224:THR:O	1:P:228:MET:HB3	2.10	0.50
1:W:248:GLU:CD	1:W:248:GLU:H	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:298:LYS:HA	1:H:301:ARG:HG2	1.94	0.50
1:S:218:HIS:CE1	1:S:285:PHE:HB2	2.45	0.50
1:B:339:THR:O	1:B:343:ILE:HG13	2.10	0.50
1:N:228:MET:HB2	1:N:267:PHE:HB3	1.93	0.50
1:Q:256:SER:HA	1:Q:259:ILE:HD12	1.94	0.50
1:T:353:GLY:O	1:T:357:ILE:HG12	2.10	0.50
1:S:288:PRO:HG3	1:S:300:LYS:HG2	1.92	0.50
1:T:250:ALA:C	1:T:252:MET:H	2.13	0.50
1:A:317:ARG:NH2	1:A:319:TYR:CD2	2.78	0.50
1:M:233:VAL:HA	1:M:243:PRO:HA	1.92	0.50
1:P:361:LEU:HG	1:P:365:LEU:HD22	1.93	0.50
1:S:218:HIS:HE1	1:S:285:PHE:HB2	1.76	0.50
1:M:297:GLY:O	1:M:301:ARG:HG3	2.12	0.50
1:S:265:LEU:HB3	1:S:266:PRO:HD3	1.94	0.50
1:G:276:GLU:CD	1:G:324:ARG:HH12	2.10	0.50
1:K:347:GLN:O	1:K:351:LEU:HD23	2.11	0.50
1:Q:204:LEU:O	1:Q:208:VAL:HG12	2.11	0.50
1:A:258:ARG:HH22	1:A:337:SER:HG	1.60	0.50
1:E:350:LYS:NZ	1:T:362:GLN:OE1	2.31	0.50
1:G:361:LEU:HG	1:G:365:LEU:HD13	1.93	0.50
1:N:304:SER:O	1:N:307:GLN:HG2	2.11	0.50
1:Q:346:ILE:O	1:Q:350:LYS:HG3	2.11	0.50
1:D:181:SER:OG	3:D:500:DAO:O1	2.25	0.50
1:D:265:LEU:O	1:D:269:GLU:HG3	2.11	0.50
1:H:205:ASP:N	1:H:205:ASP:OD1	2.42	0.50
1:J:148:GLN:HA	1:J:151:VAL:HB	1.93	0.50
1:Q:213:ALA:O	4:Q:700:HOH:O	2.20	0.50
1:S:361:LEU:HG	1:S:365:LEU:HD13	1.94	0.49
1:V:254:ARG:HA	1:V:257:ILE:HG12	1.93	0.49
1:A:272:ILE:HG23	1:A:276:GLU:HB2	1.94	0.49
1:B:354:MET:HE1	1:W:358:ASP:HB2	1.93	0.49
1:H:254:ARG:HD2	1:H:341:GLN:NE2	2.26	0.49
1:Q:208:VAL:HG21	1:T:183:LYS:HG2	1.94	0.49
1:S:177:ASP:HB3	1:S:240:TYR:CE2	2.47	0.49
1:S:279:TYR:HD2	1:S:310:LEU:HD23	1.77	0.49
1:T:352:PHE:CE2	1:T:356:LYS:HD2	2.48	0.49
1:V:234:LEU:HB3	1:V:242:VAL:HB	1.93	0.49
1:B:270:LEU:O	1:B:324:ARG:NH1	2.46	0.49
1:G:220:LEU:O	1:G:224:THR:HG22	2.11	0.49
1:M:357:ILE:HG22	1:M:358:ASP:H	1.77	0.49
1:W:273:ASP:OD2	1:W:317:ARG:NH1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:GLN:NE2	1:K:347:GLN:H	2.11	0.49
1:P:325:PHE:CZ	1:P:329:LEU:HD11	2.47	0.49
1:W:184:GLU:O	1:W:188:VAL:HG13	2.12	0.49
1:M:258:ARG:NH2	1:M:262:GLU:OE2	2.46	0.49
1:V:166:ASP:N	1:V:166:ASP:OD1	2.45	0.49
1:E:174:SER:O	1:E:178:VAL:HG23	2.11	0.49
1:K:170:LYS:HG3	1:K:241:ILE:HG23	1.93	0.49
1:P:178:VAL:HG22	1:P:236:LEU:HD11	1.93	0.49
1:Q:352:PHE:O	1:Q:356:LYS:HG3	2.12	0.49
1:K:267:PHE:HA	1:K:272:ILE:HG12	1.95	0.49
1:P:189:LEU:HD21	1:P:218:HIS:ND1	2.28	0.49
1:P:194:LYS:HA	1:P:199:PHE:CE2	2.48	0.49
1:T:325:PHE:HA	1:T:328:LEU:HD12	1.94	0.49
1:V:286:PHE:O	1:V:303:ARG:HD3	2.13	0.49
1:B:326:GLY:O	1:B:330:LEU:HG	2.13	0.49
1:G:311:GLU:HB2	1:G:325:PHE:CZ	2.48	0.49
1:H:254:ARG:HD2	1:H:341:GLN:HE22	1.78	0.49
1:P:178:VAL:HA	1:P:236:LEU:HD13	1.94	0.49
1:V:204:LEU:O	1:V:208:VAL:HG23	2.12	0.49
1:A:185:GLN:HA	1:A:188:VAL:HG22	1.95	0.48
1:A:310:LEU:O	1:A:314:ILE:HG13	2.13	0.48
1:D:308:VAL:HB	1:E:322:ARG:HE	1.78	0.48
1:H:357:ILE:O	1:H:361:LEU:HG	2.12	0.48
1:J:357:ILE:HG22	1:J:358:ASP:H	1.78	0.48
1:M:303:ARG:NE	1:N:330:LEU:HD13	2.27	0.48
1:M:307:GLN:OE1	1:N:326:GLY:HA3	2.13	0.48
1:S:297:GLY:HA2	1:S:300:LYS:HE2	1.95	0.48
1:G:185:GLN:HA	1:G:188:VAL:HG22	1.95	0.48
1:J:297:GLY:O	1:J:301:ARG:HG3	2.12	0.48
1:P:186:LEU:HD12	1:P:219:LEU:HD21	1.96	0.48
1:Q:233:VAL:HG22	1:Q:243:PRO:HA	1.94	0.48
1:N:311:GLU:OE2	1:N:315:ASN:ND2	2.46	0.48
1:V:186:LEU:HD12	1:V:219:LEU:HD21	1.95	0.48
1:B:286:PHE:O	1:B:303:ARG:HD3	2.13	0.48
1:K:351:LEU:HD13	1:K:354:MET:HE3	1.96	0.48
1:Q:295:ASP:OD2	1:Q:298:LYS:NZ	2.40	0.48
1:A:189:LEU:HD11	1:A:218:HIS:ND1	2.29	0.48
1:A:363:GLU:HG2	2:C:354:LEU:HB2	1.95	0.48
1:N:260:LEU:HD23	1:N:264:VAL:HG21	1.96	0.48
1:V:172:ILE:HG12	1:V:241:ILE:HG13	1.95	0.48
1:V:255:VAL:CG1	1:V:342:MET:HB2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:287:ASP:HB3	1:W:289:ASP:OD1	2.14	0.48
1:E:264:VAL:O	1:E:268:GLN:HG3	2.14	0.48
1:K:355:ALA:CB	1:W:351:LEU:HD11	2.43	0.48
1:M:186:LEU:HD12	1:M:219:LEU:HD21	1.96	0.48
1:P:330:LEU:HD13	1:Q:303:ARG:CZ	2.44	0.48
1:T:325:PHE:HE1	1:T:329:LEU:HD11	1.79	0.48
1:E:351:LEU:HD22	1:Q:351:LEU:HB3	1.96	0.48
1:H:170:LYS:HG2	1:H:239:ASP:HB3	1.96	0.48
1:P:327:GLU:HG3	1:Q:300:LYS:NZ	2.29	0.48
1:S:234:LEU:O	1:S:242:VAL:N	2.40	0.48
1:V:211:LEU:HD23	1:V:285:PHE:CE1	2.49	0.48
1:G:253:SER:O	1:G:257:ILE:HG13	2.13	0.48
1:J:343:ILE:O	1:J:347:GLN:HG2	2.13	0.48
1:P:243:PRO:HD2	1:P:246:CYS:SG	2.54	0.48
1:T:309:SER:HA	1:T:312:ASP:OD2	2.14	0.48
1:V:361:LEU:HG	1:V:365:LEU:HD23	1.95	0.48
1:D:279:TYR:CD2	1:D:310:LEU:HG	2.49	0.48
1:K:244:ARG:NH2	1:K:261:ASP:OD1	2.46	0.48
1:D:171:LYS:O	1:D:240:TYR:HA	2.13	0.47
1:D:318:GLN:OE1	1:V:360:LEU:HD21	2.14	0.47
1:E:255:VAL:HG11	1:E:342:MET:HE2	1.95	0.47
1:J:317:ARG:CZ	1:J:319:TYR:HB2	2.44	0.47
1:M:232:ASP:O	1:M:244:ARG:N	2.47	0.47
1:M:304:SER:O	1:M:307:GLN:HG3	2.14	0.47
1:W:245:HIS:O	1:W:247:PRO:HD3	2.15	0.47
1:B:223:ALA:HB2	3:B:500:DAO:H62	1.96	0.47
1:E:171:LYS:HG2	1:E:172:ILE:N	2.30	0.47
1:H:256:SER:HA	1:H:259:ILE:HD12	1.96	0.47
1:H:309:SER:HA	1:H:312:ASP:OD2	2.14	0.47
1:M:194:LYS:HA	1:M:199:PHE:CE2	2.49	0.47
1:M:340:TRP:CH2	1:N:337:SER:HA	2.47	0.47
1:H:178:VAL:HG11	3:H:500:DAO:H101	1.96	0.47
1:J:185:GLN:HA	1:J:188:VAL:HG22	1.96	0.47
1:J:302:LEU:O	1:J:306:VAL:HG23	2.13	0.47
1:K:173:ALA:HB2	1:K:240:TYR:HB3	1.97	0.47
1:K:199:PHE:O	1:K:207:GLN:NE2	2.45	0.47
1:W:185:GLN:O	1:W:188:VAL:HG22	2.14	0.47
1:E:265:LEU:O	1:E:269:GLU:HG3	2.13	0.47
1:M:313:TYR:CZ	1:M:317:ARG:HD2	2.49	0.47
1:Q:260:LEU:HD23	1:Q:264:VAL:HG21	1.96	0.47
1:N:317:ARG:HH12	1:N:320:ASP:C	2.18	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:354:MET:HA	1:W:357:ILE:HD12	1.96	0.47
1:A:255:VAL:O	1:A:259:ILE:HG13	2.14	0.47
1:D:276:GLU:OE1	1:D:313:TYR:HE2	1.97	0.47
1:G:273:ASP:N	1:G:276:GLU:OE2	2.44	0.47
1:W:248:GLU:OE1	1:W:248:GLU:N	2.44	0.47
1:B:255:VAL:O	1:B:259:ILE:HG13	2.15	0.47
1:G:279:TYR:HB3	1:G:310:LEU:HD12	1.97	0.47
1:J:196:ILE:HB	1:J:199:PHE:HB3	1.97	0.47
1:M:291:LYS:HG2	1:N:258:ARG:HH12	1.80	0.47
1:N:279:TYR:HE2	1:N:313:TYR:HB2	1.80	0.47
1:P:255:VAL:HG22	1:P:341:GLN:HG2	1.95	0.47
1:Q:189:LEU:HA	1:Q:192:TRP:HB3	1.97	0.47
1:T:232:ASP:HB3	1:T:244:ARG:HB2	1.97	0.47
1:T:304:SER:O	1:T:308:VAL:HG23	2.14	0.47
1:V:258:ARG:O	1:V:262:GLU:HB2	2.14	0.47
1:W:325:PHE:HA	1:W:328:LEU:HD12	1.95	0.47
1:B:325:PHE:CE1	1:B:329:LEU:HD11	2.50	0.47
1:G:364:MET:HG2	2:I:354:LEU:HD12	1.96	0.47
1:K:171:LYS:HD3	1:K:171:LYS:HA	1.62	0.47
1:N:228:MET:HB3	1:N:267:PHE:HD2	1.78	0.47
1:E:243:PRO:HD2	1:E:246:CYS:HB2	1.97	0.47
1:G:170:LYS:HB2	1:G:241:ILE:HG23	1.97	0.47
1:H:247:PRO:HA	1:H:250:ALA:HB2	1.96	0.47
1:J:244:ARG:NH1	1:J:261:ASP:OD1	2.48	0.47
1:K:361:LEU:O	1:K:365:LEU:HB2	2.15	0.47
1:S:348:PHE:HE1	1:S:352:PHE:CE2	2.33	0.47
1:T:185:GLN:O	1:T:188:VAL:HG22	2.15	0.47
1:A:171:LYS:HD2	1:A:171:LYS:HA	1.67	0.47
1:G:174:SER:O	1:G:178:VAL:HG23	2.15	0.47
1:G:330:LEU:HD13	1:H:303:ARG:HD3	1.97	0.47
1:K:365:LEU:HD23	1:N:176:ALA:HB2	1.96	0.47
1:P:181:SER:OG	1:P:237:GLY:N	2.46	0.47
1:A:174:SER:HB2	1:A:177:ASP:OD1	2.15	0.46
1:B:361:LEU:HD11	1:W:357:ILE:HD11	1.96	0.46
1:D:359:ASN:ND2	1:Q:247:PRO:HG3	2.31	0.46
1:E:185:GLN:HA	1:E:188:VAL:CG1	2.43	0.46
1:E:223:ALA:HB2	3:E:500:DAO:H32	1.97	0.46
1:E:276:GLU:OE2	1:E:317:ARG:HD2	2.14	0.46
1:G:358:ASP:OD1	1:G:359:ASN:N	2.49	0.46
1:M:314:ILE:HA	1:M:317:ARG:HB3	1.97	0.46
1:W:357:ILE:O	1:W:361:LEU:HG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:ILE:HG12	1:J:241:ILE:HD11	1.97	0.46
1:J:263:LEU:HD21	1:J:335:LEU:HD22	1.97	0.46
1:N:173:ALA:HB3	1:N:248:GLU:HG3	1.97	0.46
1:Q:233:VAL:HA	1:Q:242:VAL:O	2.14	0.46
1:W:203:PRO:O	1:W:207:GLN:HG3	2.15	0.46
1:D:280:LEU:HD11	1:D:328:LEU:HD22	1.97	0.46
1:G:149:ALA:HA	1:G:195:TYR:HB2	1.96	0.46
1:E:245:HIS:O	1:E:247:PRO:HD3	2.15	0.46
1:H:214:HIS:CE1	1:H:287:ASP:HB2	2.51	0.46
1:M:184:GLU:O	1:M:188:VAL:HG22	2.15	0.46
1:N:299:ILE:HA	1:N:302:LEU:HD12	1.97	0.46
1:P:276:GLU:O	1:P:280:LEU:HD13	2.16	0.46
1:Q:186:LEU:HD13	1:Q:186:LEU:C	2.36	0.46
1:S:316:ASP:O	1:S:321:SER:HB3	2.16	0.46
1:M:272:ILE:HG13	1:M:276:GLU:OE1	2.16	0.46
1:W:255:VAL:O	1:W:259:ILE:HG12	2.16	0.46
1:A:247:PRO:O	1:A:248:GLU:HB2	2.16	0.46
1:H:185:GLN:O	1:H:188:VAL:HG22	2.16	0.46
1:H:220:LEU:HD21	1:H:342:MET:HE1	1.98	0.46
1:S:265:LEU:O	1:S:269:GLU:HB2	2.16	0.46
1:V:282:ALA:HA	1:V:285:PHE:HB3	1.98	0.46
1:D:356:LYS:HE2	1:D:356:LYS:HB2	1.79	0.46
1:H:223:ALA:HB2	3:H:500:DAO:H32	1.97	0.46
1:J:358:ASP:OD1	1:J:359:ASN:N	2.49	0.46
1:Q:183:LYS:HD3	1:T:212:ARG:NE	2.30	0.46
1:Q:302:LEU:O	1:Q:306:VAL:HG23	2.16	0.46
1:P:295:ASP:O	1:P:299:ILE:HD12	2.16	0.46
1:P:314:ILE:HA	1:P:317:ARG:HB2	1.96	0.46
1:V:234:LEU:HD22	1:V:235:LEU:H	1.81	0.46
1:B:352:PHE:O	1:B:356:LYS:HG3	2.17	0.46
1:D:171:LYS:HG3	1:D:240:TYR:CE2	2.51	0.46
1:E:273:ASP:N	1:E:276:GLU:OE1	2.43	0.46
1:G:179:CYS:O	1:G:183:LYS:HG3	2.16	0.46
1:H:212:ARG:HG3	1:H:212:ARG:HH11	1.81	0.46
1:K:325:PHE:O	1:K:329:LEU:HG	2.15	0.46
1:V:212:ARG:NH2	1:V:363:GLU:HG3	2.25	0.46
1:A:175:ILE:HG13	1:A:176:ALA:H	1.80	0.45
1:A:279:TYR:HD2	1:A:310:LEU:HG	1.81	0.45
1:B:214:HIS:HE1	1:B:287:ASP:HB2	1.80	0.45
1:B:265:LEU:O	1:B:269:GLU:HG3	2.16	0.45
1:G:148:GLN:HE22	1:G:195:TYR:HB3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:279:TYR:HB3	1:J:310:LEU:HD11	1.97	0.45
1:K:204:LEU:HD23	1:K:207:GLN:OE1	2.16	0.45
1:N:205:ASP:OD1	1:N:205:ASP:N	2.49	0.45
1:Q:205:ASP:OD1	1:Q:205:ASP:N	2.48	0.45
1:Q:255:VAL:O	1:Q:259:ILE:HG13	2.15	0.45
1:W:297:GLY:O	1:W:301:ARG:HG3	2.16	0.45
1:M:255:VAL:O	1:M:259:ILE:HG13	2.16	0.45
1:W:178:VAL:O	1:W:182:MET:HG3	2.16	0.45
1:E:234:LEU:O	1:E:241:ILE:HA	2.16	0.45
1:J:149:ALA:HA	1:J:195:TYR:HB2	1.98	0.45
1:M:264:VAL:O	1:M:268:GLN:HG3	2.15	0.45
1:S:224:THR:HG21	1:S:263:LEU:HD22	1.98	0.45
1:W:356:LYS:HA	1:W:356:LYS:HD2	1.84	0.45
1:G:235:LEU:HD11	1:G:239:ASP:HA	1.98	0.45
1:H:231:LYS:O	1:H:233:VAL:HG12	2.15	0.45
1:W:293:LEU:HD23	1:W:293:LEU:HA	1.85	0.45
1:W:304:SER:O	1:W:307:GLN:HG2	2.16	0.45
1:E:309:SER:HA	1:E:312:ASP:OD2	2.16	0.45
1:H:252:MET:HG2	1:H:345:GLN:HG2	1.98	0.45
1:K:309:SER:HA	1:K:312:ASP:OD2	2.17	0.45
1:K:325:PHE:CE1	1:K:329:LEU:HD21	2.52	0.45
1:M:192:TRP:O	1:M:196:ILE:HG12	2.17	0.45
1:P:297:GLY:O	1:P:301:ARG:HG3	2.16	0.45
1:P:300:LYS:HE2	1:P:300:LYS:HB3	1.87	0.45
1:S:258:ARG:CZ	1:S:338:ILE:HG12	2.46	0.45
1:T:192:TRP:CZ2	1:T:196:ILE:HD11	2.52	0.45
1:A:270:LEU:O	1:A:272:ILE:N	2.49	0.45
1:B:186:LEU:O	1:B:190:VAL:HG23	2.16	0.45
1:G:264:VAL:O	1:G:268:GLN:HG3	2.16	0.45
1:M:302:LEU:O	1:M:306:VAL:HG23	2.17	0.45
1:T:243:PRO:HD2	1:T:246:CYS:HB2	1.99	0.45
1:T:255:VAL:HG11	1:T:342:MET:HE2	1.99	0.45
1:V:259:ILE:O	1:V:263:LEU:HB2	2.17	0.45
1:B:174:SER:OG	1:B:177:ASP:OD2	2.35	0.45
1:D:173:ALA:HB2	1:D:240:TYR:HB3	1.97	0.45
1:E:255:VAL:O	1:E:259:ILE:HG13	2.17	0.45
1:K:248:GLU:OE1	1:K:248:GLU:N	2.36	0.45
1:M:312:ASP:OD1	1:N:322:ARG:NH1	2.50	0.45
1:N:264:VAL:HG12	1:N:268:GLN:HE21	1.81	0.45
1:N:309:SER:HA	1:N:312:ASP:OD2	2.17	0.45
1:Q:230:PHE:HE2	1:Q:235:LEU:HD22	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:352:PHE:O	1:W:356:LYS:HG2	2.16	0.45
1:D:307:GLN:HE21	1:E:323:GLY:HA2	1.81	0.45
1:G:310:LEU:HD21	1:G:328:LEU:HD13	1.98	0.45
1:T:340:TRP:HA	1:T:343:ILE:HG12	1.98	0.45
1:V:185:GLN:HB3	1:V:219:LEU:HD22	1.98	0.45
1:V:317:ARG:H	1:V:321:SER:HB3	1.81	0.45
1:W:344:GLU:O	1:W:348:PHE:HB2	2.17	0.45
1:A:307:GLN:HE21	1:A:308:VAL:CG2	2.29	0.45
1:H:176:ALA:O	1:H:180:GLU:HG3	2.17	0.45
1:N:324:ARG:O	1:N:328:LEU:HG	2.17	0.45
1:W:181:SER:HB2	1:W:238:ASN:ND2	2.31	0.45
1:B:270:LEU:HB3	1:B:324:ARG:HH12	1.82	0.45
1:B:304:SER:O	1:B:307:GLN:HG3	2.16	0.45
1:E:185:GLN:HG3	3:E:500:DAO:H21	1.98	0.45
1:G:350:LYS:NZ	1:T:250:ALA:HB3	2.32	0.45
1:N:181:SER:HA	1:N:184:GLU:HG2	1.99	0.45
1:P:218:HIS:CE1	1:P:285:PHE:HB2	2.52	0.45
1:S:186:LEU:CD1	1:S:219:LEU:HD11	2.47	0.45
1:B:303:ARG:HA	1:B:306:VAL:HG12	1.98	0.44
1:D:302:LEU:O	1:D:306:VAL:HG23	2.17	0.44
1:T:324:ARG:O	1:T:328:LEU:HG	2.17	0.44
1:T:340:TRP:O	1:T:343:ILE:HG12	2.17	0.44
1:V:341:GLN:O	1:V:345:GLN:HG2	2.17	0.44
1:A:243:PRO:HD2	1:A:246:CYS:SG	2.57	0.44
1:A:339:THR:O	1:A:343:ILE:HG13	2.18	0.44
1:G:350:LYS:HD3	1:T:250:ALA:HB3	2.00	0.44
1:J:183:LYS:HE2	1:J:358:ASP:HB2	1.99	0.44
1:P:286:PHE:O	1:P:303:ARG:HD2	2.17	0.44
1:B:234:LEU:O	1:B:241:ILE:HA	2.18	0.44
1:N:279:TYR:CD2	1:N:310:LEU:HA	2.52	0.44
1:P:265:LEU:O	1:P:269:GLU:HG3	2.18	0.44
1:V:206:ASP:CG	1:V:294:SER:H	2.20	0.44
1:D:167:ILE:HA	1:D:170:LYS:HD2	1.97	0.44
1:G:336:GLN:HE22	1:H:337:SER:HB2	1.83	0.44
1:H:267:PHE:CD2	1:H:272:ILE:HD12	2.53	0.44
1:J:147:LEU:O	1:J:151:VAL:HG23	2.17	0.44
1:N:265:LEU:HB3	1:N:266:PRO:HD3	1.99	0.44
1:S:189:LEU:HD21	1:S:218:HIS:ND1	2.32	0.44
1:S:204:LEU:O	1:S:208:VAL:HG23	2.18	0.44
1:T:175:ILE:HG22	1:T:179:CYS:SG	2.57	0.44
1:W:205:ASP:N	1:W:205:ASP:OD1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:HE3	1:A:291:LYS:HB3	1.74	0.44
1:E:194:LYS:HE2	1:H:191:GLU:OE1	2.18	0.44
1:E:272:ILE:HD12	1:E:328:LEU:HD21	1.98	0.44
1:G:175:ILE:HG13	1:G:176:ALA:H	1.83	0.44
1:G:184:GLU:O	1:G:188:VAL:HG13	2.18	0.44
1:N:279:TYR:HB2	1:N:310:LEU:HD23	2.00	0.44
1:Q:322:ARG:HA	1:Q:322:ARG:NE	2.32	0.44
1:T:235:LEU:HD11	1:T:239:ASP:HA	1.99	0.44
1:A:170:LYS:HD3	1:A:241:ILE:HG21	1.99	0.44
1:G:173:ALA:HB2	1:G:240:TYR:HB3	1.99	0.44
1:N:346:ILE:O	1:N:350:LYS:HG3	2.18	0.44
1:V:310:LEU:HD13	1:V:314:ILE:HD12	1.99	0.44
1:A:184:GLU:O	1:A:188:VAL:HG13	2.17	0.44
1:D:173:ALA:HA	1:D:240:TYR:HD2	1.82	0.44
1:K:192:TRP:O	1:K:195:TYR:HB2	2.18	0.44
1:P:325:PHE:O	1:P:328:LEU:HB2	2.17	0.44
1:Q:325:PHE:HA	1:Q:328:LEU:HD12	2.00	0.44
1:S:326:GLY:O	1:S:330:LEU:HG	2.18	0.44
1:V:174:SER:O	1:V:178:VAL:HG23	2.18	0.44
1:E:231:LYS:O	1:E:233:VAL:HG12	2.17	0.44
1:G:347:GLN:OE1	1:G:366:LEU:HD13	2.18	0.44
1:K:348:PHE:CE2	1:W:348:PHE:CZ	3.06	0.44
1:P:264:VAL:O	1:P:268:GLN:HG3	2.18	0.44
1:P:341:GLN:O	1:P:345:GLN:HG2	2.16	0.44
1:A:357:ILE:HG22	1:A:358:ASP:H	1.83	0.44
1:H:351:LEU:HD11	1:T:355:ALA:HB2	2.00	0.44
1:K:265:LEU:O	1:K:269:GLU:HG3	2.18	0.44
1:P:253:SER:O	1:P:257:ILE:HG13	2.18	0.44
1:V:235:LEU:HD11	1:V:239:ASP:HA	2.00	0.44
1:H:350:LYS:HG3	1:H:354:MET:CE	2.45	0.43
1:K:245:HIS:O	1:K:247:PRO:HD3	2.17	0.43
1:M:311:GLU:HB2	1:M:325:PHE:CE2	2.53	0.43
1:P:224:THR:HG1	1:P:267:PHE:HE2	1.63	0.43
1:P:361:LEU:HA	1:P:365:LEU:HD13	2.00	0.43
1:B:177:ASP:O	1:B:238:ASN:ND2	2.50	0.43
1:D:254:ARG:O	1:D:258:ARG:HG3	2.18	0.43
1:N:233:VAL:HA	1:N:242:VAL:O	2.18	0.43
1:W:324:ARG:O	1:W:328:LEU:HG	2.18	0.43
1:J:217:GLU:OE1	1:J:339:THR:HG21	2.19	0.43
1:J:293:LEU:HB2	1:J:296:PRO:HG3	2.00	0.43
1:J:350:LYS:NZ	1:W:250:ALA:HB3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:311:GLU:HB2	1:K:325:PHE:HE2	1.84	0.43
1:T:184:GLU:O	1:T:188:VAL:HG13	2.17	0.43
1:A:185:GLN:HG3	3:A:500:DAO:O2	2.18	0.43
1:E:173:ALA:HB2	1:E:240:TYR:HB3	2.01	0.43
1:K:284:ILE:HG23	1:K:332:LEU:HD22	2.00	0.43
1:Q:226:ARG:HG2	1:Q:235:LEU:HD23	2.00	0.43
1:S:174:SER:OG	1:S:175:ILE:N	2.52	0.43
1:S:303:ARG:NE	1:T:330:LEU:HD13	2.34	0.43
1:T:205:ASP:N	1:T:205:ASP:OD1	2.51	0.43
1:J:175:ILE:HD12	1:J:355:ALA:HB2	2.01	0.43
1:K:325:PHE:CE1	1:K:329:LEU:HD11	2.54	0.43
1:B:264:VAL:O	1:B:268:GLN:HG3	2.19	0.43
1:E:356:LYS:HD3	1:P:344:GLU:OE2	2.19	0.43
1:G:356:LYS:HD2	1:T:248:GLU:HG3	2.01	0.43
1:K:304:SER:O	1:K:307:GLN:HG3	2.17	0.43
1:N:345:GLN:O	1:N:349:ILE:HG12	2.19	0.43
1:T:181:SER:HB2	1:T:238:ASN:HD21	1.83	0.43
1:D:224:THR:HG21	1:D:263:LEU:HB3	2.00	0.43
1:E:187:LEU:HD21	1:H:211:LEU:HD22	1.99	0.43
1:K:364:MET:CB	1:V:254:ARG:HH22	2.32	0.43
1:M:181:SER:OG	1:M:236:LEU:HB3	2.19	0.43
1:P:182:MET:O	1:P:186:LEU:HB2	2.18	0.43
1:S:173:ALA:HB2	1:S:240:TYR:CB	2.48	0.43
1:W:265:LEU:HB3	1:W:266:PRO:HD3	2.01	0.43
1:B:173:ALA:HA	1:B:240:TYR:HD2	1.84	0.43
1:N:204:LEU:O	1:N:208:VAL:HG23	2.18	0.43
1:S:253:SER:O	1:S:257:ILE:HG13	2.18	0.43
1:B:270:LEU:HB3	1:B:324:ARG:NH1	2.34	0.43
1:D:174:SER:O	1:D:178:VAL:HG23	2.18	0.43
1:D:359:ASN:CB	2:F:353:GLU:HB2	2.49	0.43
1:E:263:LEU:O	1:E:267:PHE:HD2	2.02	0.43
1:N:255:VAL:O	1:N:259:ILE:HG13	2.19	0.43
1:Q:260:LEU:HA	1:Q:264:VAL:CG2	2.48	0.43
1:V:179:CYS:O	1:V:182:MET:HG2	2.18	0.43
1:B:362:GLN:O	1:B:366:LEU:N	2.41	0.43
1:E:186:LEU:O	1:E:190:VAL:HG23	2.19	0.43
1:H:361:LEU:HA	1:H:364:MET:HG2	2.00	0.43
1:N:204:LEU:HB3	1:W:184:GLU:HG2	2.01	0.43
1:N:276:GLU:O	1:N:280:LEU:HB2	2.19	0.43
1:Q:265:LEU:HB3	1:Q:266:PRO:HD3	2.01	0.43
1:W:274:ASP:HA	1:W:277:TYR:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:O	1:A:258:ARG:HB2	2.18	0.42
1:E:349:ILE:HA	1:E:352:PHE:HD1	1.84	0.42
1:G:330:LEU:HD23	1:G:330:LEU:HA	1.89	0.42
1:H:248:GLU:CD	1:H:248:GLU:H	2.22	0.42
1:J:174:SER:O	1:J:178:VAL:HG23	2.19	0.42
1:J:182:MET:HG2	3:J:500:DAO:H22	2.01	0.42
1:J:307:GLN:NE2	1:K:327:GLU:OE1	2.47	0.42
1:K:224:THR:HG23	1:K:264:VAL:HG22	2.00	0.42
1:K:297:GLY:O	1:K:301:ARG:HG3	2.19	0.42
1:M:171:LYS:HD3	1:M:240:TYR:HE1	1.83	0.42
1:M:308:VAL:HG22	1:N:323:GLY:HA2	2.01	0.42
1:N:353:GLY:O	1:N:357:ILE:HG13	2.19	0.42
1:P:186:LEU:HD13	1:P:219:LEU:HD11	2.01	0.42
1:V:317:ARG:H	1:V:321:SER:CB	2.31	0.42
1:A:218:HIS:NE2	1:A:281:LYS:O	2.52	0.42
1:D:276:GLU:OE1	1:D:276:GLU:N	2.52	0.42
1:E:192:TRP:CE2	1:E:281:LYS:HD3	2.54	0.42
1:Q:181:SER:HA	1:Q:184:GLU:HG2	2.01	0.42
1:A:363:GLU:HG2	2:C:354:LEU:CB	2.49	0.42
1:D:270:LEU:HB3	1:D:324:ARG:NH1	2.35	0.42
1:G:234:LEU:HB2	1:G:242:VAL:HB	2.02	0.42
1:Q:184:GLU:O	1:Q:188:VAL:HG13	2.18	0.42
1:S:174:SER:O	1:S:178:VAL:HG23	2.19	0.42
1:S:324:ARG:NH1	1:S:328:LEU:HD11	2.34	0.42
1:T:217:GLU:O	1:T:221:LEU:HG	2.19	0.42
1:T:224:THR:O	1:T:228:MET:HB3	2.19	0.42
1:T:339:THR:O	1:T:343:ILE:HG23	2.19	0.42
1:B:356:LYS:NZ	1:M:344:GLU:O	2.53	0.42
1:E:349:ILE:HG23	1:E:352:PHE:HE1	1.84	0.42
1:K:264:VAL:O	1:K:268:GLN:HG3	2.19	0.42
1:P:171:LYS:HA	1:P:171:LYS:HD2	1.66	0.42
1:W:309:SER:HA	1:W:312:ASP:OD2	2.19	0.42
1:D:143:ILE:HD13	1:D:279:TYR:CE1	2.55	0.42
1:D:178:VAL:HG22	1:D:236:LEU:HD11	2.01	0.42
1:H:173:ALA:HB1	1:H:177:ASP:HB2	2.02	0.42
1:H:207:GLN:O	1:H:211:LEU:HD13	2.19	0.42
1:J:262:GLU:HG2	1:K:289:ASP:CG	2.39	0.42
1:N:177:ASP:HA	1:N:180:GLU:HB3	2.01	0.42
1:N:186:LEU:HA	1:N:219:LEU:HD21	2.02	0.42
1:N:243:PRO:HD2	1:N:246:CYS:HB2	2.02	0.42
1:T:345:GLN:HA	1:T:348:PHE:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ALA:O	1:A:252:MET:SD	2.77	0.42
1:A:357:ILE:HG22	1:A:358:ASP:N	2.35	0.42
1:D:175:ILE:HG13	1:D:176:ALA:H	1.83	0.42
1:D:236:LEU:HD22	3:D:500:DAO:H42	2.02	0.42
1:H:192:TRP:O	1:H:195:TYR:HB2	2.19	0.42
1:K:228:MET:O	1:K:268:GLN:HG2	2.19	0.42
1:N:304:SER:O	1:N:308:VAL:HG23	2.19	0.42
1:Q:191:GLU:OE2	1:T:190:VAL:HG12	2.19	0.42
1:S:213:ALA:O	1:S:214:HIS:ND1	2.49	0.42
1:W:291:LYS:H	1:W:291:LYS:HD2	1.83	0.42
1:J:267:PHE:CD1	1:J:272:ILE:HD12	2.55	0.42
1:S:348:PHE:HE1	1:S:352:PHE:HE2	1.67	0.42
1:A:229:VAL:HG23	1:A:230:PHE:CD1	2.55	0.42
1:G:325:PHE:CZ	1:G:329:LEU:HD11	2.54	0.42
1:H:175:ILE:HD13	1:H:249:LEU:CD2	2.50	0.42
1:K:311:GLU:HB2	1:K:325:PHE:CE2	2.55	0.42
1:N:231:LYS:HD2	1:N:268:GLN:HE22	1.85	0.42
1:A:279:TYR:CD2	1:A:310:LEU:HG	2.55	0.42
1:A:359:ASN:CG	1:N:247:PRO:HG3	2.40	0.42
1:G:148:GLN:O	1:G:151:VAL:HB	2.20	0.42
1:J:175:ILE:HG13	1:J:176:ALA:H	1.85	0.42
1:J:353:GLY:HA3	1:W:175:ILE:HG12	2.02	0.42
1:Q:242:VAL:CG1	1:Q:249:LEU:HD21	2.49	0.42
1:T:178:VAL:O	1:T:182:MET:HG3	2.20	0.42
1:D:179:CYS:HB3	1:D:183:LYS:NZ	2.35	0.42
1:H:325:PHE:CE1	1:H:329:LEU:HD11	2.54	0.42
1:T:192:TRP:HH2	1:T:285:PHE:CE2	2.38	0.42
1:T:352:PHE:O	1:T:356:LYS:HG3	2.20	0.42
1:E:217:GLU:HB3	1:E:335:LEU:HD21	2.02	0.41
1:J:212:ARG:NH2	1:J:291:LYS:HZ1	2.18	0.41
1:V:255:VAL:O	1:V:259:ILE:HG13	2.19	0.41
1:D:255:VAL:O	1:D:259:ILE:HG13	2.20	0.41
1:G:255:VAL:O	1:G:259:ILE:HG13	2.21	0.41
1:G:281:LYS:O	1:G:285:PHE:HB2	2.20	0.41
1:H:304:SER:O	1:H:307:GLN:HG3	2.19	0.41
1:N:302:LEU:O	1:N:306:VAL:HG23	2.20	0.41
1:P:257:ILE:HG13	1:P:257:ILE:H	1.67	0.41
1:T:357:ILE:O	1:T:361:LEU:HG	2.19	0.41
1:A:297:GLY:O	1:A:301:ARG:HG3	2.20	0.41
1:A:310:LEU:HD23	1:A:313:TYR:HD2	1.84	0.41
1:B:279:TYR:CD2	1:B:310:LEU:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ALA:HB2	3:D:500:DAO:H31	2.03	0.41
1:M:303:ARG:NH2	1:N:330:LEU:HB3	2.36	0.41
1:P:185:GLN:CD	1:P:219:LEU:HD22	2.40	0.41
1:P:232:ASP:O	1:P:244:ARG:N	2.53	0.41
1:P:340:TRP:CH2	1:Q:337:SER:HA	2.56	0.41
1:Q:322:ARG:HE	1:Q:323:GLY:H	1.69	0.41
1:Q:346:ILE:HG22	1:Q:350:LYS:HE3	2.02	0.41
1:A:186:LEU:HD11	1:A:365:LEU:CD1	2.51	0.41
1:E:232:ASP:CG	1:E:244:ARG:HE	2.23	0.41
1:G:174:SER:OG	1:G:177:ASP:OD1	2.22	0.41
1:G:357:ILE:H	1:T:248:GLU:CD	2.24	0.41
1:Q:186:LEU:CD2	1:Q:215:ALA:HB1	2.50	0.41
1:S:357:ILE:HG22	1:S:358:ASP:N	2.35	0.41
1:B:238:ASN:OD1	1:B:238:ASN:N	2.46	0.41
1:D:229:VAL:HG23	1:D:230:PHE:CD1	2.55	0.41
1:E:232:ASP:OD1	1:E:244:ARG:NH2	2.48	0.41
1:G:196:ILE:HB	1:G:199:PHE:HB3	2.02	0.41
1:N:230:PHE:HB3	1:N:233:VAL:HG23	2.02	0.41
1:P:231:LYS:O	1:P:233:VAL:HG23	2.20	0.41
1:Q:190:VAL:HG22	1:Q:211:LEU:HD13	2.02	0.41
1:Q:228:MET:HB2	1:Q:267:PHE:HB3	2.03	0.41
1:S:330:LEU:HD13	1:T:303:ARG:NE	2.35	0.41
1:V:213:ALA:O	1:V:214:HIS:ND1	2.49	0.41
1:D:167:ILE:O	1:D:170:LYS:HB2	2.21	0.41
1:D:225:LYS:HD2	1:D:277:TYR:CE2	2.56	0.41
1:H:234:LEU:O	1:H:241:ILE:HA	2.20	0.41
1:H:351:LEU:HA	1:H:354:MET:SD	2.61	0.41
1:J:258:ARG:NE	1:J:262:GLU:OE2	2.38	0.41
1:M:213:ALA:O	1:M:214:HIS:ND1	2.47	0.41
1:P:216:GLY:O	1:P:220:LEU:HD23	2.21	0.41
1:P:260:LEU:O	1:P:264:VAL:HG12	2.21	0.41
1:Q:204:LEU:HB3	1:T:184:GLU:HG2	2.01	0.41
1:V:300:LYS:O	1:V:304:SER:OG	2.39	0.41
1:V:327:GLU:HB2	1:W:307:GLN:HE22	1.85	0.41
1:W:313:TYR:O	1:W:317:ARG:HG3	2.20	0.41
1:J:255:VAL:HG11	3:J:500:DAO:H101	2.03	0.41
1:M:289:ASP:HB3	1:N:262:GLU:OE1	2.20	0.41
1:S:288:PRO:O	1:S:293:LEU:HD12	2.20	0.41
1:S:327:GLU:HA	1:S:330:LEU:HD12	2.02	0.41
1:T:210:LEU:HD23	1:T:210:LEU:HA	1.82	0.41
1:A:304:SER:O	1:A:307:GLN:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:GLN:O	1:D:348:PHE:HB3	2.20	0.41
1:J:167:ILE:HB	1:J:168:ARG:NH1	2.36	0.41
1:J:222:GLY:O	1:J:226:ARG:HG3	2.21	0.41
1:J:341:GLN:O	1:J:345:GLN:HG3	2.20	0.41
1:K:209:ALA:HB1	1:K:291:LYS:O	2.20	0.41
1:K:310:LEU:O	1:K:314:ILE:HG12	2.21	0.41
1:P:253:SER:O	1:P:256:SER:OG	2.25	0.41
1:P:290:ALA:HB3	1:P:293:LEU:HG	2.03	0.41
1:P:323:GLY:O	1:Q:307:GLN:NE2	2.54	0.41
1:S:286:PHE:O	1:S:303:ARG:HD3	2.21	0.41
1:V:212:ARG:O	1:V:212:ARG:HG2	2.21	0.41
1:A:236:LEU:HD12	1:A:240:TYR:HB2	2.02	0.41
1:B:189:LEU:C	1:B:189:LEU:CD2	2.88	0.41
1:G:357:ILE:HG22	1:G:358:ASP:N	2.35	0.41
1:H:214:HIS:O	1:H:218:HIS:HD2	2.03	0.41
1:J:185:GLN:HA	1:J:188:VAL:CG2	2.51	0.41
1:J:291:LYS:O	1:J:291:LYS:NZ	2.46	0.41
1:K:326:GLY:O	1:K:330:LEU:HG	2.20	0.41
1:M:170:LYS:HB2	1:M:241:ILE:HD13	2.02	0.41
1:Q:279:TYR:HB2	1:Q:310:LEU:HD23	2.03	0.41
1:S:272:ILE:HG23	1:S:276:GLU:OE1	2.21	0.41
1:E:331:LEU:O	1:E:334:THR:OG1	2.26	0.41
1:H:234:LEU:N	1:H:242:VAL:O	2.49	0.41
1:N:259:ILE:HG23	1:N:263:LEU:HD12	2.03	0.41
1:N:360:LEU:O	1:N:364:MET:HG2	2.21	0.41
1:S:226:ARG:CD	1:S:237:GLY:HA2	2.50	0.41
1:V:302:LEU:O	1:V:306:VAL:HG23	2.21	0.41
1:D:300:LYS:HE2	1:D:300:LYS:HB3	1.93	0.40
1:J:150:GLU:N	1:J:192:TRP:HD1	2.18	0.40
1:J:205:ASP:O	1:J:208:VAL:HG12	2.20	0.40
1:N:233:VAL:HG12	1:N:243:PRO:HA	2.03	0.40
1:N:254:ARG:H	1:N:254:ARG:HG2	1.51	0.40
1:P:330:LEU:HD13	1:Q:303:ARG:NE	2.37	0.40
1:T:265:LEU:HB3	1:T:266:PRO:HD3	2.04	0.40
1:A:187:LEU:HA	1:A:190:VAL:HG12	2.04	0.40
1:A:226:ARG:NH2	1:A:235:LEU:O	2.45	0.40
1:Q:300:LYS:HA	1:Q:300:LYS:HD2	1.84	0.40
1:T:317:ARG:HB3	1:T:317:ARG:NH1	2.36	0.40
1:Q:186:LEU:HD21	1:Q:215:ALA:HB1	2.04	0.40
1:S:229:VAL:HG23	1:S:230:PHE:CD1	2.57	0.40
1:S:252:MET:SD	1:S:252:MET:N	2.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:302:LEU:O	1:S:306:VAL:HG23	2.22	0.40
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.81	0.40
1:G:350:LYS:HZ2	1:T:250:ALA:HB3	1.86	0.40
1:J:339:THR:O	1:J:343:ILE:HG13	2.21	0.40
1:W:346:ILE:HG13	1:W:346:ILE:H	1.71	0.40
1:A:143:ILE:HA	1:A:146:LEU:HD12	2.04	0.40
1:B:288:PRO:HG3	1:B:300:LYS:HG2	2.03	0.40
1:D:321:SER:OG	1:D:321:SER:O	2.38	0.40
1:G:307:GLN:HE22	1:H:323:GLY:HA2	1.86	0.40
1:J:186:LEU:CD1	1:J:219:LEU:HD11	2.52	0.40
1:K:325:PHE:CD1	1:K:329:LEU:HD11	2.56	0.40
1:P:248:GLU:HG3	1:P:249:LEU:HG	2.04	0.40
1:S:308:VAL:HA	1:S:311:GLU:HB3	2.04	0.40

All (2) 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:240:TYR:OH	1:T:316:ASP:O[2_544]	2.15	0.05
1:A:171:LYS:NZ	1:W:316:ASP:O[2_445]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/245 (84%)	189 (92%)	17 (8%)	0	100	100
1	B	203/245 (83%)	189 (93%)	13 (6%)	1 (0%)	29	66
1	D	210/245 (86%)	190 (90%)	18 (9%)	2 (1%)	15	52
1	E	202/245 (82%)	190 (94%)	12 (6%)	0	100	100
1	G	205/245 (84%)	182 (89%)	23 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	200/245 (82%)	192 (96%)	7 (4%)	1 (0%)	29 66
1	J	205/245 (84%)	187 (91%)	17 (8%)	1 (0%)	29 66
1	K	200/245 (82%)	185 (92%)	15 (8%)	0	100 100
1	M	199/245 (81%)	178 (89%)	20 (10%)	1 (0%)	29 66
1	N	191/245 (78%)	186 (97%)	5 (3%)	0	100 100
1	P	198/245 (81%)	178 (90%)	20 (10%)	0	100 100
1	Q	194/245 (79%)	183 (94%)	11 (6%)	0	100 100
1	S	199/245 (81%)	173 (87%)	24 (12%)	2 (1%)	15 52
1	T	190/245 (78%)	181 (95%)	9 (5%)	0	100 100
1	V	200/245 (82%)	181 (90%)	19 (10%)	0	100 100
1	W	190/245 (78%)	179 (94%)	11 (6%)	0	100 100
2	C	5/20 (25%)	5 (100%)	0	0	100 100
2	F	5/20 (25%)	5 (100%)	0	0	100 100
2	I	5/20 (25%)	5 (100%)	0	0	100 100
2	L	6/20 (30%)	6 (100%)	0	0	100 100
All	All	3213/4000 (80%)	2964 (92%)	241 (8%)	8 (0%)	47 78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	321	SER
1	M	318	GLN
1	S	248	GLU
1	H	232	ASP
1	B	232	ASP
1	D	248	GLU
1	D	247	PRO
1	S	318	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/214 (86%)	178 (96%)	7 (4%)	33 66
1	B	181/214 (85%)	177 (98%)	4 (2%)	52 78
1	D	188/214 (88%)	182 (97%)	6 (3%)	39 70
1	E	180/214 (84%)	178 (99%)	2 (1%)	73 88
1	G	184/214 (86%)	180 (98%)	4 (2%)	52 78
1	H	179/214 (84%)	176 (98%)	3 (2%)	60 82
1	J	184/214 (86%)	178 (97%)	6 (3%)	38 70
1	K	179/214 (84%)	175 (98%)	4 (2%)	52 78
1	M	178/214 (83%)	171 (96%)	7 (4%)	32 65
1	N	172/214 (80%)	169 (98%)	3 (2%)	60 82
1	P	177/214 (83%)	169 (96%)	8 (4%)	27 61
1	Q	175/214 (82%)	173 (99%)	2 (1%)	73 88
1	S	177/214 (83%)	170 (96%)	7 (4%)	31 64
1	T	172/214 (80%)	169 (98%)	3 (2%)	60 82
1	V	179/214 (84%)	173 (97%)	6 (3%)	37 69
1	W	172/214 (80%)	169 (98%)	3 (2%)	60 82
2	C	5/17 (29%)	4 (80%)	1 (20%)	1 6
2	F	5/17 (29%)	5 (100%)	0	100 100
2	I	5/17 (29%)	5 (100%)	0	100 100
2	L	6/17 (35%)	6 (100%)	0	100 100
All	All	2883/3492 (83%)	2807 (97%)	76 (3%)	46 75

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ASP
1	A	221	LEU
1	A	307	GLN
1	A	317	ARG
1	A	337	SER
1	A	348	PHE
1	A	362	GLN
1	B	164	ASN
1	B	166	ASP
1	B	305	GLN
1	B	325	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	353	GLU
1	D	152	LEU
1	D	177	ASP
1	D	252	MET
1	D	276	GLU
1	D	307	GLN
1	D	348	PHE
1	E	318	GLN
1	E	325	PHE
1	G	177	ASP
1	G	221	LEU
1	G	307	GLN
1	G	362	GLN
1	H	303	ARG
1	H	315	ASN
1	H	325	PHE
1	J	147	LEU
1	J	177	ASP
1	J	307	GLN
1	J	337	SER
1	J	340	TRP
1	J	362	GLN
1	K	315	ASN
1	K	316	ASP
1	K	325	PHE
1	K	348	PHE
1	M	177	ASP
1	M	221	LEU
1	M	252	MET
1	M	307	GLN
1	M	318	GLN
1	M	348	PHE
1	M	364	MET
1	N	174	SER
1	N	325	PHE
1	N	348	PHE
1	P	177	ASP
1	P	179	CYS
1	P	221	LEU
1	P	252	MET
1	P	307	GLN
1	P	319	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	348	PHE
1	P	362	GLN
1	Q	254	ARG
1	Q	325	PHE
1	S	177	ASP
1	S	221	LEU
1	S	252	MET
1	S	267	PHE
1	S	307	GLN
1	S	319	TYR
1	S	348	PHE
1	T	199	PHE
1	T	315	ASN
1	T	325	PHE
1	V	177	ASP
1	V	221	LEU
1	V	252	MET
1	V	307	GLN
1	V	313	TYR
1	V	362	GLN
1	W	244	ARG
1	W	254	ARG
1	W	325	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	268	GLN
1	G	336	GLN
1	J	207	GLN
1	K	347	GLN
2	L	359	GLN
1	M	268	GLN
1	N	268	GLN
1	N	307	GLN
1	P	307	GLN
1	Q	185	GLN
1	T	307	GLN
1	V	207	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 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	DAO	H	500	1	13,13,13	0.65	0	13,13,13	1.23	1 (7%)
3	DAO	J	500	-	13,13,13	0.64	0	13,13,13	1.21	1 (7%)
3	DAO	D	500	-	13,13,13	0.62	0	13,13,13	1.14	0
3	DAO	G	500	1	13,13,13	0.64	0	13,13,13	1.18	1 (7%)
3	DAO	K	500	1	13,13,13	0.59	0	13,13,13	1.10	0
3	DAO	A	500	1	13,13,13	0.63	0	13,13,13	1.14	0
3	DAO	B	500	1	13,13,13	0.65	0	13,13,13	1.29	1 (7%)
3	DAO	E	500	1	13,13,13	0.64	0	13,13,13	1.27	1 (7%)

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	DAO	H	500	1	-	4/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAO	J	500	-	-	7/11/11/11	-
3	DAO	D	500	-	-	6/11/11/11	-
3	DAO	G	500	1	-	2/11/11/11	-
3	DAO	K	500	1	-	7/11/11/11	-
3	DAO	A	500	1	-	3/11/11/11	-
3	DAO	B	500	1	-	3/11/11/11	-
3	DAO	E	500	1	-	3/11/11/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	500	DAO	C3-C2-C1	-2.76	107.51	114.47
3	E	500	DAO	C3-C2-C1	-2.74	107.56	114.47
3	J	500	DAO	C3-C2-C1	-2.47	108.24	114.47
3	H	500	DAO	C3-C2-C1	-2.34	108.57	114.47
3	G	500	DAO	O2-C1-C2	2.15	120.94	114.03

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	500	DAO	C1-C2-C3-C4
3	J	500	DAO	C1-C2-C3-C4
3	B	500	DAO	C2-C3-C4-C5
3	B	500	DAO	C5-C6-C7-C8
3	J	500	DAO	C3-C4-C5-C6
3	K	500	DAO	C2-C3-C4-C5
3	D	500	DAO	C6-C7-C8-C9
3	K	500	DAO	C5-C6-C7-C8
3	K	500	DAO	C4-C5-C6-C7
3	E	500	DAO	C5-C6-C7-C8
3	K	500	DAO	C3-C4-C5-C6
3	B	500	DAO	C11-C10-C9-C8
3	A	500	DAO	C6-C7-C8-C9
3	D	500	DAO	C2-C3-C4-C5
3	J	500	DAO	C9-C10-C11-C12
3	K	500	DAO	C6-C7-C8-C9
3	H	500	DAO	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	500	DAO	C2-C3-C4-C5
3	G	500	DAO	C7-C8-C9-C10
3	K	500	DAO	C1-C2-C3-C4
3	A	500	DAO	O2-C1-C2-C3
3	D	500	DAO	O1-C1-C2-C3
3	J	500	DAO	C6-C7-C8-C9
3	A	500	DAO	O1-C1-C2-C3
3	J	500	DAO	O2-C1-C2-C3
3	H	500	DAO	C7-C8-C9-C10
3	J	500	DAO	O1-C1-C2-C3
3	D	500	DAO	O2-C1-C2-C3
3	H	500	DAO	O2-C1-C2-C3
3	E	500	DAO	C9-C10-C11-C12
3	J	500	DAO	C5-C6-C7-C8
3	H	500	DAO	O1-C1-C2-C3
3	D	500	DAO	C7-C8-C9-C10
3	E	500	DAO	C3-C4-C5-C6
3	K	500	DAO	O2-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	500	DAO	2	0
3	J	500	DAO	2	0
3	D	500	DAO	3	0
3	G	500	DAO	3	0
3	K	500	DAO	1	0
3	A	500	DAO	1	0
3	B	500	DAO	2	0
3	E	500	DAO	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	210/245 (85%)	1.08	35 (16%)	1	1	18, 46, 87, 107	0
1	B	205/245 (83%)	0.72	20 (9%)	7	4	12, 28, 86, 118	0
1	D	214/245 (87%)	1.30	43 (20%)	1	0	73, 127, 199, 208	0
1	E	204/245 (83%)	1.08	24 (11%)	4	2	85, 120, 145, 157	0
1	G	209/245 (85%)	0.98	36 (17%)	1	1	63, 95, 117, 128	0
1	H	202/245 (82%)	1.00	26 (12%)	3	2	25, 62, 101, 124	0
1	J	209/245 (85%)	0.97	32 (15%)	2	1	41, 70, 103, 141	0
1	K	202/245 (82%)	0.76	16 (7%)	12	6	18, 40, 81, 99	0
1	M	201/245 (82%)	2.53	97 (48%)	0	0	84, 193, 319, 333	0
1	N	193/245 (78%)	2.31	88 (45%)	0	0	58, 207, 454, 485	0
1	P	200/245 (81%)	2.47	97 (48%)	0	0	118, 152, 235, 277	0
1	Q	196/245 (80%)	2.39	85 (43%)	0	0	69, 209, 377, 395	0
1	S	201/245 (82%)	1.55	62 (30%)	0	0	69, 139, 198, 244	0
1	T	192/245 (78%)	1.51	60 (31%)	0	0	101, 153, 174, 180	0
1	V	202/245 (82%)	1.67	70 (34%)	0	0	89, 129, 164, 192	0
1	W	192/245 (78%)	1.60	57 (29%)	0	0	54, 142, 162, 167	0
2	C	7/20 (35%)	1.77	1 (14%)	2	1	76, 79, 90, 95	0
2	F	7/20 (35%)	1.39	1 (14%)	2	1	127, 137, 150, 152	0
2	I	7/20 (35%)	1.58	2 (28%)	0	0	188, 189, 191, 191	0
2	L	8/20 (40%)	2.11	3 (37%)	0	0	84, 87, 89, 92	0
All	All	3261/4000 (81%)	1.49	855 (26%)	0	0	12, 120, 260, 485	0

All (855) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	280	LEU	16.7
1	M	316	ASP	14.8
1	M	315	ASN	14.7
1	A	320	ASP	13.0
1	P	280	LEU	12.7
1	M	329	LEU	12.1
1	Q	286	PHE	11.1
1	P	221	LEU	11.0
1	P	200	CYS	11.0
1	N	329	LEU	10.6
1	D	151	VAL	10.4
1	N	268	GLN	10.4
1	A	151	VAL	10.2
1	M	169	ALA	10.0
1	N	196	ILE	9.9
1	Q	195	TYR	9.9
1	N	195	TYR	9.7
1	Q	282	ALA	9.4
1	N	286	PHE	8.9
1	P	203	PRO	8.9
1	Q	193	ALA	8.8
1	M	173	ALA	8.4
1	S	274	ASP	8.3
1	Q	285	PHE	8.2
1	Q	306	VAL	8.2
1	Q	284	ILE	8.2
1	V	272	ILE	7.8
1	S	293	LEU	7.8
1	S	286	PHE	7.6
1	M	319	TYR	7.5
1	S	328	LEU	7.5
1	M	167	ILE	7.5
1	P	275	ASN	7.5
1	W	197	PRO	7.5
1	P	195	TYR	7.4
1	M	331	LEU	7.4
1	P	259	ILE	7.4
1	N	331	LEU	7.4
1	P	179	CYS	7.3
1	N	247	PRO	7.3
1	Q	223	ALA	7.3
1	Q	172	ILE	7.3
1	Q	331	LEU	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	329	LEU	7.2
1	M	233	VAL	7.2
1	P	297	GLY	7.2
1	Q	196	ILE	7.0
1	V	271	GLN	7.0
2	C	356	ALA	7.0
1	N	326	GLY	7.0
1	W	191	GLU	6.9
1	N	323	GLY	6.9
1	V	286	PHE	6.8
1	T	191	GLU	6.8
1	T	197	PRO	6.8
1	P	191	GLU	6.7
1	W	248	GLU	6.7
1	S	327	GLU	6.6
1	N	285	PHE	6.6
1	Q	316	ASP	6.6
1	E	268	GLN	6.6
1	M	326	GLY	6.6
1	P	274	ASP	6.6
1	T	209	ALA	6.6
1	G	362	GLN	6.6
1	M	191	GLU	6.5
1	Q	299	ILE	6.5
1	P	299	ILE	6.5
1	P	222	GLY	6.5
1	J	146	LEU	6.4
1	Q	283	ILE	6.4
1	Q	221	LEU	6.4
1	N	283	ILE	6.3
1	Q	301	ARG	6.3
2	L	357	LEU	6.3
1	N	282	ALA	6.3
1	S	271	GLN	6.2
1	Q	277	TYR	6.2
1	W	215	ALA	6.2
1	V	274	ASP	6.2
1	P	233	VAL	6.1
1	V	327	GLU	6.1
1	V	264	VAL	6.1
1	W	286	PHE	6.1
1	W	280	LEU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	322	ARG	6.0
1	E	233	VAL	6.0
1	Q	338	ILE	6.0
1	V	230	PHE	6.0
1	P	250	ALA	6.0
1	P	173	ALA	5.9
1	M	247	PRO	5.9
1	M	195	TYR	5.9
1	P	316	ASP	5.9
1	Q	332	LEU	5.8
1	N	193	ALA	5.8
1	V	288	PRO	5.8
1	V	277	TYR	5.8
1	Q	227	SER	5.8
1	V	330	LEU	5.7
1	T	200	CYS	5.7
1	N	188	VAL	5.7
1	Q	330	LEU	5.7
1	N	218	HIS	5.7
1	N	246	CYS	5.7
1	T	242	VAL	5.7
1	M	218	HIS	5.7
1	P	331	LEU	5.7
1	N	293	LEU	5.6
1	W	219	LEU	5.6
1	M	258	ARG	5.6
1	N	315	ASN	5.6
1	V	294	SER	5.6
1	M	259	ILE	5.6
1	M	179	CYS	5.6
1	Q	194	LYS	5.6
1	P	305	GLN	5.6
1	Q	247	PRO	5.5
1	N	330	LEU	5.5
1	S	232	ASP	5.5
1	M	297	GLY	5.5
1	Q	329	LEU	5.5
1	V	166	ASP	5.4
1	M	279	TYR	5.4
1	M	287	ASP	5.4
1	Q	268	GLN	5.3
1	V	322	ARG	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	299	ILE	5.3
1	N	284	ILE	5.3
1	Q	201	GLU	5.3
2	F	356	ALA	5.3
1	M	170	LYS	5.2
1	G	243	PRO	5.2
1	A	304	SER	5.2
1	Q	279	TYR	5.2
1	A	213	ALA	5.2
1	N	227	SER	5.2
1	Q	333	PRO	5.2
1	N	221	LEU	5.2
1	M	275	ASN	5.2
1	S	277	TYR	5.2
1	S	272	ILE	5.2
1	M	256	SER	5.1
1	W	218	HIS	5.1
1	G	239	ASP	5.1
1	N	301	ARG	5.1
1	M	221	LEU	5.1
1	V	206	ASP	5.1
1	W	222	GLY	5.1
1	D	247	PRO	5.0
1	J	362	GLN	5.0
1	D	207	GLN	5.0
1	S	288	PRO	5.0
1	W	209	ALA	5.0
1	P	218	HIS	5.0
1	M	312	ASP	5.0
1	Q	347	GLN	5.0
1	M	328	LEU	5.0
1	N	257	ILE	4.9
1	M	248	GLU	4.9
1	D	320	ASP	4.9
1	W	281	LYS	4.8
1	V	306	VAL	4.8
1	K	244	ARG	4.8
1	T	307	GLN	4.8
1	B	268	GLN	4.8
1	E	271	GLN	4.8
1	S	323	GLY	4.8
1	T	274	ASP	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	217	GLU	4.7
1	J	286	PHE	4.7
1	T	287	ASP	4.7
1	G	286	PHE	4.7
1	P	340	TRP	4.7
1	T	215	ALA	4.7
1	H	315	ASN	4.7
1	V	328	LEU	4.7
1	N	338	ILE	4.7
1	Q	235	LEU	4.7
2	L	353	GLU	4.7
1	P	312	ASP	4.7
1	S	206	ASP	4.7
1	N	253	SER	4.6
1	N	228	MET	4.6
1	Q	294	SER	4.6
1	T	222	GLY	4.6
1	V	167	ILE	4.6
1	N	340	TRP	4.6
1	P	314	ILE	4.6
1	V	326	GLY	4.6
1	M	322	ARG	4.6
1	A	318	GLN	4.5
1	T	324	ARG	4.5
1	S	319	TYR	4.5
1	K	217	GLU	4.5
1	J	191	GLU	4.5
1	P	279	TYR	4.5
1	P	192	TRP	4.5
1	S	322	ARG	4.4
1	D	282	ALA	4.4
1	J	347	GLN	4.4
1	G	172	ILE	4.4
1	V	252	MET	4.4
1	N	316	ASP	4.4
1	J	250	ALA	4.4
1	W	324	ARG	4.4
1	J	243	PRO	4.4
1	V	211	LEU	4.4
1	P	209	ALA	4.4
1	H	216	GLY	4.4
1	P	282	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	323	GLY	4.3
1	W	278	ALA	4.3
1	S	312	ASP	4.3
1	P	201	GLU	4.3
2	I	353	GLU	4.3
1	P	267	PHE	4.3
1	D	166	ASP	4.3
1	Q	303	ARG	4.3
1	T	319	TYR	4.3
1	V	363	GLU	4.3
1	A	150	GLU	4.3
1	S	358	ASP	4.3
1	W	245	HIS	4.3
1	M	267	PHE	4.2
1	V	324	ARG	4.2
1	N	190	VAL	4.2
1	W	319	TYR	4.2
1	P	296	PRO	4.2
1	Q	295	ASP	4.2
1	N	265	LEU	4.2
1	V	229	VAL	4.2
1	M	274	ASP	4.2
1	N	336	GLN	4.2
1	W	292	GLY	4.2
1	M	340	TRP	4.2
1	S	368	GLY	4.2
1	M	200	CYS	4.2
1	A	294	SER	4.2
1	P	202	LEU	4.2
1	V	318	GLN	4.2
1	Q	320	ASP	4.2
1	P	322	ARG	4.1
1	T	303	ARG	4.1
1	P	223	ALA	4.1
1	P	239	ASP	4.1
1	V	250	ALA	4.1
1	D	367	GLY	4.1
1	W	190	VAL	4.1
1	P	238	ASN	4.1
1	G	250	ALA	4.1
1	W	316	ASP	4.1
1	A	319	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	278	ALA	4.1
1	V	312	ASP	4.1
1	E	187	LEU	4.1
1	V	320	ASP	4.1
1	E	340	TRP	4.1
1	N	303	ARG	4.0
1	V	293	LEU	4.0
1	S	230	PHE	4.0
1	J	145	ALA	4.0
1	P	315	ASN	4.0
1	P	323	GLY	4.0
1	W	289	ASP	4.0
1	S	363	GLU	4.0
1	H	280	LEU	4.0
1	N	325	PHE	4.0
1	E	276	GLU	3.9
1	J	195	TYR	3.9
1	Q	188	VAL	3.9
1	P	256	SER	3.9
1	P	287	ASP	3.9
1	N	251	GLU	3.9
1	B	249	LEU	3.9
1	N	291	LYS	3.9
1	P	170	LYS	3.9
1	T	234	LEU	3.9
1	W	198	ALA	3.9
1	T	281	LYS	3.9
1	W	264	VAL	3.9
1	G	152	LEU	3.9
1	M	325	PHE	3.9
1	W	283	ILE	3.9
1	H	359	ASN	3.9
1	M	246	CYS	3.9
1	K	216	GLY	3.9
1	N	351	LEU	3.9
1	P	273	ASP	3.9
1	N	182	MET	3.9
1	Q	257	ILE	3.9
1	N	287	ASP	3.9
1	H	304	SER	3.9
1	W	186	LEU	3.9
1	K	318	GLN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	259	ILE	3.9
1	J	354	MET	3.9
1	K	224	THR	3.9
1	T	280	LEU	3.9
1	V	232	ASP	3.9
1	S	330	LEU	3.8
1	M	216	GLY	3.8
1	V	217	GLU	3.8
1	Q	234	LEU	3.8
1	T	278	ALA	3.8
1	W	249	LEU	3.8
1	J	172	ILE	3.8
1	P	246	CYS	3.8
1	Q	351	LEU	3.8
1	P	216	GLY	3.8
1	T	214	HIS	3.8
1	W	234	LEU	3.8
1	D	251	GLU	3.8
1	V	263	LEU	3.8
1	T	217	GLU	3.8
1	W	282	ALA	3.8
1	D	213	ALA	3.7
1	N	194	LYS	3.7
1	W	214	HIS	3.7
1	J	148	GLN	3.7
1	M	318	GLN	3.7
1	P	330	LEU	3.7
1	Q	334	THR	3.7
1	V	195	TYR	3.7
1	D	150	GLU	3.7
1	V	323	GLY	3.7
1	D	360	LEU	3.7
1	T	239	ASP	3.7
1	M	250	ALA	3.7
1	W	242	VAL	3.7
1	P	346	ILE	3.7
1	B	340	TRP	3.7
1	N	235	LEU	3.7
1	N	279	TYR	3.7
1	T	327	GLU	3.6
1	N	229	VAL	3.6
1	G	294	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	270	LEU	3.6
1	M	199	PHE	3.6
1	N	203	PRO	3.6
1	S	291	LYS	3.6
1	W	309	SER	3.6
1	M	186	LEU	3.6
1	M	257	ILE	3.6
1	P	247	PRO	3.5
1	Q	203	PRO	3.5
1	N	314	ILE	3.5
1	W	322	ARG	3.5
1	T	289	ASP	3.5
1	K	215	ALA	3.5
1	N	321	SER	3.5
1	A	152	LEU	3.5
1	S	211	LEU	3.5
1	S	254	ARG	3.5
1	V	273	ASP	3.5
1	W	307	GLN	3.5
1	M	225	LYS	3.5
1	P	252	MET	3.5
1	P	281	LYS	3.5
1	S	264	VAL	3.5
1	D	280	LEU	3.5
1	Q	207	GLN	3.5
1	M	192	TRP	3.5
1	T	248	GLU	3.5
1	T	258	ARG	3.5
1	S	262	GLU	3.4
1	P	294	SER	3.4
1	Q	246	CYS	3.4
1	G	146	LEU	3.4
1	K	256	SER	3.4
1	V	309	SER	3.4
1	S	311	GLU	3.4
1	D	318	GLN	3.4
1	Q	253	SER	3.4
1	N	269	GLU	3.4
1	Q	337	SER	3.4
1	H	175	ILE	3.4
1	D	272	ILE	3.4
1	B	276	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	233	VAL	3.4
1	M	237	GLY	3.4
1	Q	228	MET	3.4
1	P	317	ARG	3.4
1	J	221	LEU	3.4
1	J	271	GLN	3.4
1	M	222	GLY	3.3
1	B	166	ASP	3.3
1	G	306	VAL	3.3
1	P	214	HIS	3.3
1	Q	315	ASN	3.3
1	W	359	ASN	3.3
1	Q	319	TYR	3.3
1	P	225	LYS	3.3
1	B	235	LEU	3.3
1	V	265	LEU	3.3
1	S	268	GLN	3.3
1	Q	313	TYR	3.3
1	N	223	ALA	3.3
1	T	249	LEU	3.3
1	H	245	HIS	3.3
1	N	189	LEU	3.3
1	N	277	TYR	3.3
1	M	296	PRO	3.2
1	M	346	ILE	3.2
1	T	219	LEU	3.2
1	P	342	MET	3.2
1	D	219	LEU	3.2
1	P	197	PRO	3.2
1	W	271	GLN	3.2
1	Q	300	LYS	3.2
1	H	244	ARG	3.2
1	S	283	ILE	3.2
1	N	319	TYR	3.2
1	A	245	HIS	3.2
1	T	283	ILE	3.2
1	P	198	ALA	3.2
1	P	199	PHE	3.2
1	Q	214	HIS	3.2
1	M	278	ALA	3.2
1	P	230	PHE	3.2
1	P	266	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	W	303	ARG	3.2
1	E	235	LEU	3.2
1	N	332	LEU	3.1
1	Q	241	ILE	3.1
1	S	247	PRO	3.1
1	V	249	LEU	3.1
1	N	297	GLY	3.1
1	W	233	VAL	3.1
1	Q	291	LYS	3.1
1	V	283	ILE	3.1
1	M	305	GLN	3.1
1	V	282	ALA	3.1
1	P	301	ARG	3.1
1	Q	181	SER	3.1
1	G	191	GLU	3.1
1	A	298	LYS	3.1
1	W	239	ASP	3.1
1	P	186	LEU	3.1
1	E	194	LYS	3.1
1	S	195	TYR	3.1
1	G	354	MET	3.1
1	S	188	VAL	3.1
1	W	315	ASN	3.1
1	N	320	ASP	3.0
1	W	308	VAL	3.0
1	G	267	PHE	3.0
1	J	249	LEU	3.0
1	T	270	LEU	3.0
1	P	169	ALA	3.0
1	B	237	GLY	3.0
1	Q	190	VAL	3.0
1	T	309	SER	3.0
1	M	266	PRO	3.0
1	T	218	HIS	3.0
1	V	191	GLU	3.0
1	A	280	LEU	3.0
1	P	227	SER	3.0
1	N	333	PRO	3.0
2	I	357	LEU	3.0
1	T	315	ASN	3.0
1	T	190	VAL	3.0
1	M	330	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	316	ASP	3.0
1	W	312	ASP	3.0
1	G	268	GLN	3.0
1	P	205	ASP	3.0
1	P	313	TYR	3.0
1	S	351	LEU	3.0
1	K	198	ALA	3.0
1	D	287	ASP	3.0
1	T	264	VAL	3.0
1	B	364	MET	3.0
1	N	262	GLU	2.9
1	N	334	THR	2.9
1	E	329	LEU	2.9
1	M	281	LYS	2.9
1	V	313	TYR	2.9
1	G	145	ALA	2.9
1	S	313	TYR	2.9
1	M	317	ARG	2.9
1	N	201	GLU	2.9
1	V	258	ARG	2.9
1	T	322	ARG	2.9
1	N	275	ASN	2.9
1	T	188	VAL	2.9
1	S	250	ALA	2.9
1	S	212	ARG	2.9
1	V	357	ILE	2.9
1	D	307	GLN	2.9
1	T	207	GLN	2.9
1	W	327	GLU	2.9
1	S	294	SER	2.9
1	G	312	ASP	2.9
1	P	326	GLY	2.9
1	T	285	PHE	2.9
1	J	351	LEU	2.9
1	P	193	ALA	2.8
1	S	317	ARG	2.8
1	M	241	ILE	2.8
1	H	174	SER	2.8
1	A	307	GLN	2.8
1	H	198	ALA	2.8
1	M	277	TYR	2.8
1	V	215	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	367	GLY	2.8
1	A	247	PRO	2.8
1	M	342	MET	2.8
1	H	224	THR	2.8
1	J	167	ILE	2.8
1	M	240	TYR	2.8
1	P	268	GLN	2.8
1	A	232	ASP	2.8
1	J	235	LEU	2.8
1	N	302	LEU	2.8
1	M	303	ARG	2.8
1	D	199	PHE	2.8
1	T	316	ASP	2.8
1	V	173	ALA	2.8
1	M	238	ASN	2.8
1	N	252	MET	2.8
1	A	366	LEU	2.8
1	H	204	LEU	2.8
1	M	321	SER	2.8
1	Q	275	ASN	2.8
1	T	238	ASN	2.8
1	Q	218	HIS	2.8
1	T	286	PHE	2.8
1	G	211	LEU	2.7
1	E	176	ALA	2.7
1	M	197	PRO	2.7
1	T	233	VAL	2.7
1	N	212	ARG	2.7
1	D	321	SER	2.7
1	P	229	VAL	2.7
1	T	325	PHE	2.7
1	A	259	ILE	2.7
1	M	196	ILE	2.7
1	M	338	ILE	2.7
1	V	275	ASN	2.7
1	W	272	ILE	2.7
1	P	196	ILE	2.7
1	B	227	SER	2.7
1	K	271	GLN	2.7
1	Q	302	LEU	2.7
1	T	271	GLN	2.7
1	Q	340	TRP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	337	SER	2.7
1	D	238	ASN	2.7
1	E	283	ILE	2.7
1	P	338	ILE	2.7
1	N	234	LEU	2.7
1	M	207	GLN	2.7
1	P	336	GLN	2.7
1	M	203	PRO	2.7
1	N	328	LEU	2.7
1	G	148	GLN	2.7
1	V	311	GLU	2.7
1	D	263	LEU	2.7
1	G	184	GLU	2.7
1	E	249	LEU	2.6
1	Q	192	TRP	2.6
1	V	303	ARG	2.6
1	A	295	ASP	2.6
1	N	266	PRO	2.6
1	S	292	GLY	2.6
1	P	288	PRO	2.6
1	S	174	SER	2.6
1	A	282	ALA	2.6
1	D	260	LEU	2.6
1	N	248	GLU	2.6
1	D	340	TRP	2.6
1	K	315	ASN	2.6
1	W	274	ASP	2.6
1	P	210	LEU	2.6
1	S	279	TYR	2.6
1	Q	318	GLN	2.6
1	S	265	LEU	2.6
1	M	212	ARG	2.6
1	M	324	ARG	2.6
1	H	200	CYS	2.6
1	M	211	LEU	2.6
1	A	303	ARG	2.6
1	V	321	SER	2.6
1	D	264	VAL	2.6
1	V	201	GLU	2.6
1	V	291	LYS	2.6
1	M	214	HIS	2.6
1	A	309	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	322	ARG	2.6
1	G	195	TYR	2.6
1	N	318	GLN	2.6
1	Q	248	GLU	2.6
1	S	249	LEU	2.6
1	A	199	PHE	2.5
1	W	275	ASN	2.5
1	D	215	ALA	2.5
1	N	264	VAL	2.5
1	V	255	VAL	2.5
1	V	239	ASP	2.5
1	V	247	PRO	2.5
1	E	193	ALA	2.5
1	M	345	GLN	2.5
1	M	208	VAL	2.5
1	B	187	LEU	2.5
1	B	329	LEU	2.5
1	E	196	ILE	2.5
1	M	219	LEU	2.5
1	W	194	LYS	2.5
1	P	251	GLU	2.5
1	G	292	GLY	2.5
1	W	341	GLN	2.5
1	B	206	ASP	2.5
1	N	358	ASP	2.5
1	Q	287	ASP	2.5
1	V	243	PRO	2.5
1	E	250	ALA	2.5
1	J	237	GLY	2.5
1	J	353	GLY	2.5
1	Q	335	LEU	2.5
1	B	292	GLY	2.5
1	M	239	ASP	2.5
1	Q	206	ASP	2.5
1	A	218	HIS	2.5
1	G	328	LEU	2.5
1	T	275	ASN	2.5
1	E	232	ASP	2.5
1	M	333	PRO	2.5
1	S	278	ALA	2.5
1	W	188	VAL	2.5
1	E	225	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	351	LEU	2.5
1	W	323	GLY	2.5
1	Q	349	ILE	2.5
1	N	260	LEU	2.5
1	V	242	VAL	2.5
1	M	320	ASP	2.5
1	Q	296	PRO	2.5
1	T	312	ASP	2.5
1	H	176	ALA	2.5
1	D	205	ASP	2.5
1	N	274	ASP	2.5
1	E	337	SER	2.5
1	W	285	PHE	2.4
1	H	311	GLU	2.4
1	P	278	ALA	2.4
1	A	219	LEU	2.4
1	P	248	GLU	2.4
1	Q	197	PRO	2.4
1	M	220	LEU	2.4
1	P	220	LEU	2.4
1	D	267	PHE	2.4
1	S	309	SER	2.4
1	V	319	TYR	2.4
1	P	194	LYS	2.4
1	Q	336	GLN	2.4
1	V	268	GLN	2.4
1	N	270	LEU	2.4
1	H	313	TYR	2.4
1	N	241	ILE	2.4
1	T	359	ASN	2.4
1	T	208	VAL	2.4
1	W	247	PRO	2.4
1	D	277	TYR	2.4
1	Q	321	SER	2.4
1	B	228	MET	2.4
1	P	190	VAL	2.4
1	G	223	ALA	2.4
1	S	282	ALA	2.4
1	A	272	ILE	2.4
1	T	304	SER	2.4
1	M	229	VAL	2.4
1	P	362	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	188	VAL	2.4
1	D	276	GLU	2.4
1	S	251	GLU	2.4
1	N	280	LEU	2.4
1	V	351	LEU	2.4
1	K	304	SER	2.4
1	S	318	GLN	2.4
1	H	215	ALA	2.4
1	P	255	VAL	2.4
1	S	224	THR	2.4
1	S	324	ARG	2.3
1	N	347	GLN	2.3
1	P	240	TYR	2.3
1	B	194	LYS	2.3
1	M	232	ASP	2.3
1	V	174	SER	2.3
1	S	236	LEU	2.3
1	M	336	GLN	2.3
1	Q	182	MET	2.3
1	A	241	ILE	2.3
1	D	242	VAL	2.3
1	M	262	GLU	2.3
1	Q	276	GLU	2.3
1	J	239	ASP	2.3
1	G	235	LEU	2.3
1	T	223	ALA	2.3
1	V	299	ILE	2.3
1	T	308	VAL	2.3
1	S	182	MET	2.3
1	V	182	MET	2.3
1	B	365	LEU	2.3
2	L	355	LYS	2.3
1	S	242	VAL	2.3
1	M	174	SER	2.3
1	M	227	SER	2.3
1	D	245	HIS	2.3
1	H	223	ALA	2.3
1	J	209	ALA	2.3
1	H	292	GLY	2.3
1	P	353	GLY	2.3
1	M	294	SER	2.3
1	N	342	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	W	192	TRP	2.3
1	J	312	ASP	2.3
1	P	277	TYR	2.3
1	E	216	GLY	2.3
1	G	279	TYR	2.3
1	N	349	ILE	2.3
1	M	308	VAL	2.3
1	H	297	GLY	2.3
1	W	184	GLU	2.3
1	G	197	PRO	2.3
1	A	220	LEU	2.3
1	H	236	LEU	2.3
1	Q	328	LEU	2.3
1	D	148	GLN	2.3
1	N	214	HIS	2.3
1	W	340	TRP	2.3
1	A	251	GLU	2.3
1	J	206	ASP	2.3
1	W	220	LEU	2.3
1	P	325	PHE	2.3
1	M	201	GLU	2.3
1	Q	251	GLU	2.3
1	Q	353	GLY	2.3
1	K	263	LEU	2.3
1	Q	342	MET	2.3
1	A	149	ALA	2.3
1	P	318	GLN	2.3
1	W	207	GLN	2.3
1	A	367	GLY	2.2
1	G	206	ASP	2.2
1	W	287	ASP	2.2
1	P	208	VAL	2.2
1	B	271	GLN	2.2
1	E	180	GLU	2.2
1	D	142	SER	2.2
1	E	234	LEU	2.2
1	G	364	MET	2.2
1	Q	261	ASP	2.2
1	D	303	ARG	2.2
1	Q	187	LEU	2.2
1	P	359	ASN	2.2
1	Q	229	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	168	ARG	2.2
1	A	148	GLN	2.2
1	H	336	GLN	2.2
1	D	294	SER	2.2
1	V	364	MET	2.2
1	H	344	GLU	2.2
1	V	278	ALA	2.2
1	P	328	LEU	2.2
1	V	260	LEU	2.2
1	A	364	MET	2.2
1	E	190	VAL	2.2
1	A	197	PRO	2.2
1	A	207	GLN	2.2
1	J	186	LEU	2.2
1	S	275	ASN	2.2
1	S	349	ILE	2.2
1	P	219	LEU	2.2
1	T	317	ARG	2.2
1	N	352	PHE	2.2
1	M	354	MET	2.2
1	T	184	GLU	2.2
1	W	260	LEU	2.2
1	N	176	ALA	2.2
1	N	335	LEU	2.2
1	P	212	ARG	2.2
1	Q	317	ARG	2.2
1	S	258	ARG	2.2
1	D	271	GLN	2.2
1	J	289	ASP	2.2
1	T	243	PRO	2.2
1	S	243	PRO	2.2
1	J	266	PRO	2.1
1	K	295	ASP	2.1
1	T	323	GLY	2.1
1	P	324	ARG	2.1
1	G	274	ASP	2.1
1	T	348	PHE	2.1
1	N	296	PRO	2.1
1	B	366	LEU	2.1
1	E	206	ASP	2.1
1	Q	310	LEU	2.1
1	M	298	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	282	ALA	2.1
1	H	326	GLY	2.1
1	M	273	ASP	2.1
1	M	313	TYR	2.1
1	Q	269	GLU	2.1
1	E	172	ILE	2.1
1	J	268	GLN	2.1
1	P	241	ILE	2.1
1	T	211	LEU	2.1
1	T	247	PRO	2.1
1	N	317	ARG	2.1
1	V	194	LYS	2.1
1	Q	173	ALA	2.1
1	S	201	GLU	2.1
1	S	306	VAL	2.1
1	M	334	THR	2.1
1	T	305	GLN	2.1
1	J	147	LEU	2.1
1	K	366	LEU	2.1
1	D	206	ASP	2.1
1	N	278	ALA	2.1
1	N	313	TYR	2.1
1	B	275	ASN	2.1
1	H	234	LEU	2.1
1	D	243	PRO	2.1
1	Q	262	GLU	2.1
1	A	205	ASP	2.1
1	G	208	VAL	2.1
1	J	357	ILE	2.1
1	M	360	LEU	2.1
1	P	168	ARG	2.1
1	W	180	GLU	2.1
1	S	229	VAL	2.1
1	N	353	GLY	2.1
1	P	319	TYR	2.1
1	J	208	VAL	2.1
1	M	301	ARG	2.1
1	S	209	ALA	2.1
1	T	255	VAL	2.1
1	D	249	LEU	2.1
1	G	271	GLN	2.0
1	G	347	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	289	ASP	2.1
1	S	226	ARG	2.0
1	D	329	LEU	2.0
1	G	171	LYS	2.0
1	M	288	PRO	2.0
1	G	295	ASP	2.0
1	K	202	LEU	2.0
1	V	338	ILE	2.0
1	P	339	THR	2.0
1	G	305	GLN	2.0
1	J	251	GLU	2.0
1	M	309	SER	2.0
1	D	359	ASN	2.0
1	V	344	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DAO	G	500	14/14	0.52	0.69	75,96,103,105	0
3	DAO	J	500	14/14	0.56	0.90	62,80,95,96	0
3	DAO	D	500	14/14	0.64	0.56	78,95,114,119	0
3	DAO	K	500	14/14	0.69	0.51	15,34,44,48	0
3	DAO	H	500	14/14	0.71	0.59	41,45,54,56	0
3	DAO	A	500	14/14	0.76	0.36	42,52,70,74	0
3	DAO	B	500	14/14	0.83	0.41	21,26,46,47	0
3	DAO	E	500	14/14	0.87	0.41	94,108,118,119	0

6.5 Other polymers (i)

There are no such residues in this entry.