



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1POY
Title : SPERMIDINE/PUTRESCINE-BINDING PROTEIN COMPLEXED WITH SPERMIDINE (DIMER FORM)
Authors : Sugiyama, S.; Vassilyev, D.G.; Matsushima, M.; Morikawa, K.
Deposited on : 1996-02-02
Resolution : 2.50 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

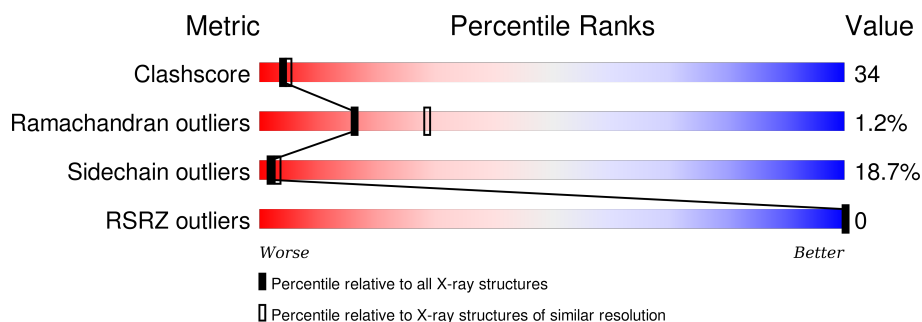
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




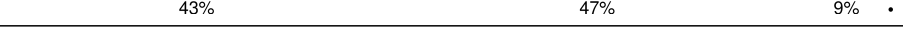
The reported resolution of this entry is 2.50 Å.

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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1	323	
1	2	323	
1	3	323	
1	4	323	

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
2	SPD	1	400	-	-	X	-
2	SPD	2	400	-	-	X	X
2	SPD	4	400	-	-	-	X

2 Entry composition [i](#)

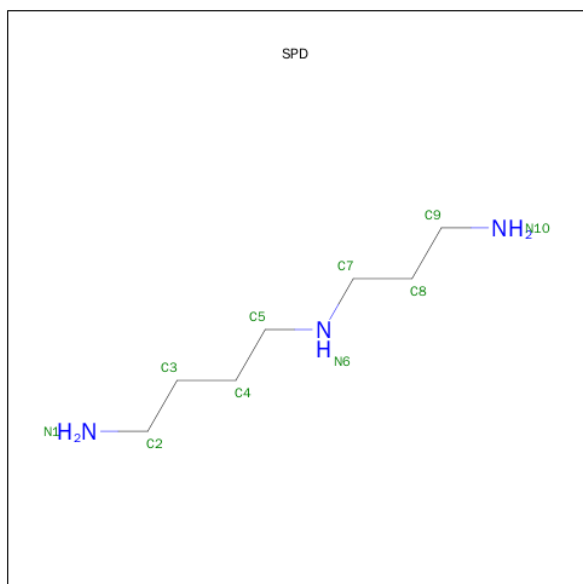
There are 3 unique types of molecules in this entry. The entry contains 10512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SPERMIDINE/PUTRESCINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	323	Total	C	N	O	S	0	0	0
			2557	1642	412	494	9			
1	2	323	Total	C	N	O	S	0	0	0
			2560	1643	412	496	9			
1	3	323	Total	C	N	O	S	0	0	0
			2560	1643	412	496	9			
1	4	323	Total	C	N	O	S	0	0	0
			2560	1643	412	496	9			

- Molecule 2 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1	1	Total	C	N	0	0
			10	7	3		
2	2	1	Total	C	N	0	0
			10	7	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	3	1	Total	C	N	0	0
			10	7	3		
2	4	1	Total	C	N	0	0
			10	7	3		

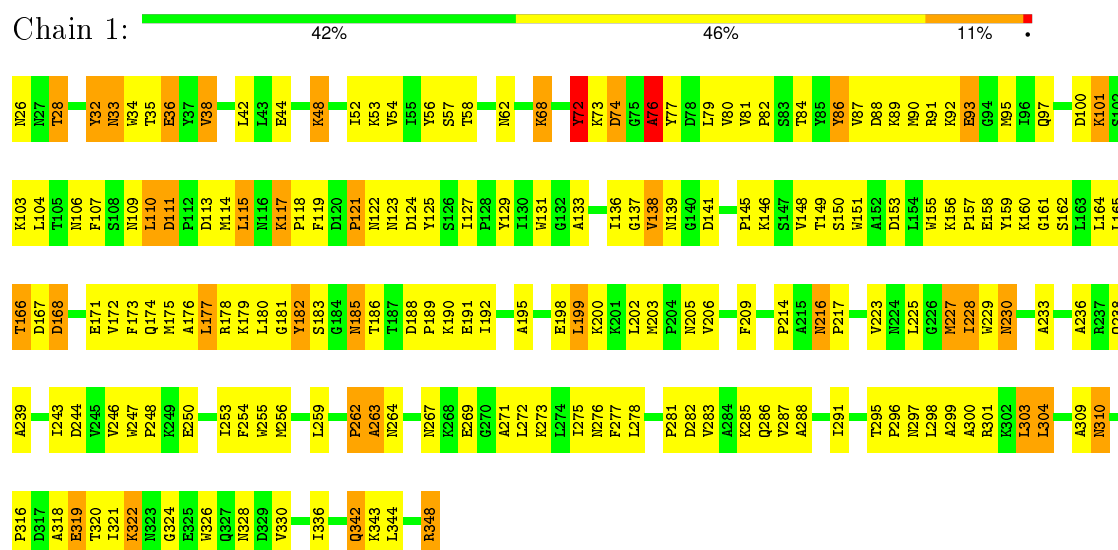
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	59	Total	O	0	0
			59	59		
3	2	53	Total	O	0	0
			53	53		
3	3	71	Total	O	0	0
			71	71		
3	4	52	Total	O	0	0
			52	52		

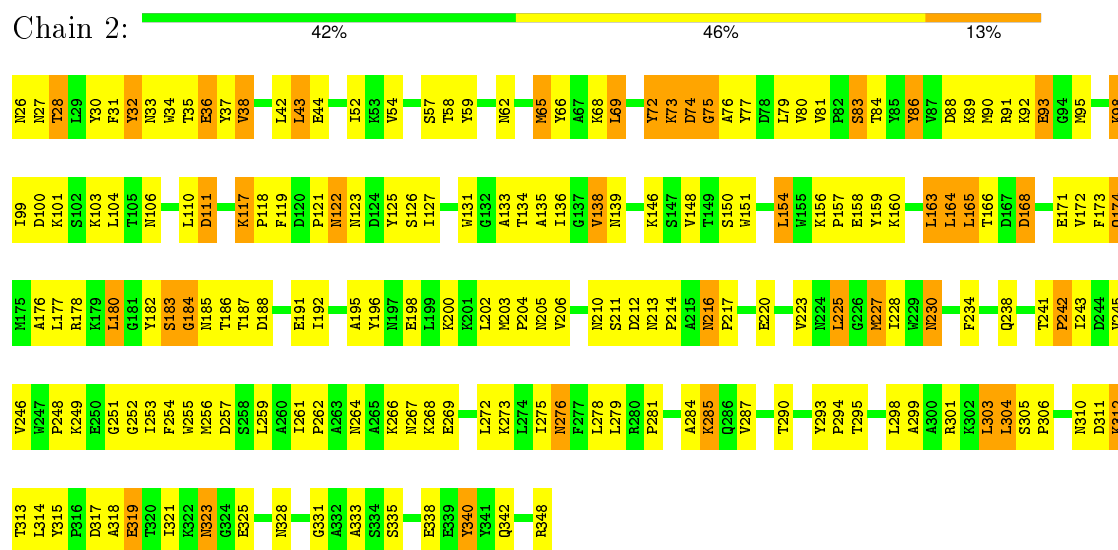
3 Residue-property plots

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: SPERMIDINE/PUTRESCINE-BINDING PROTEIN

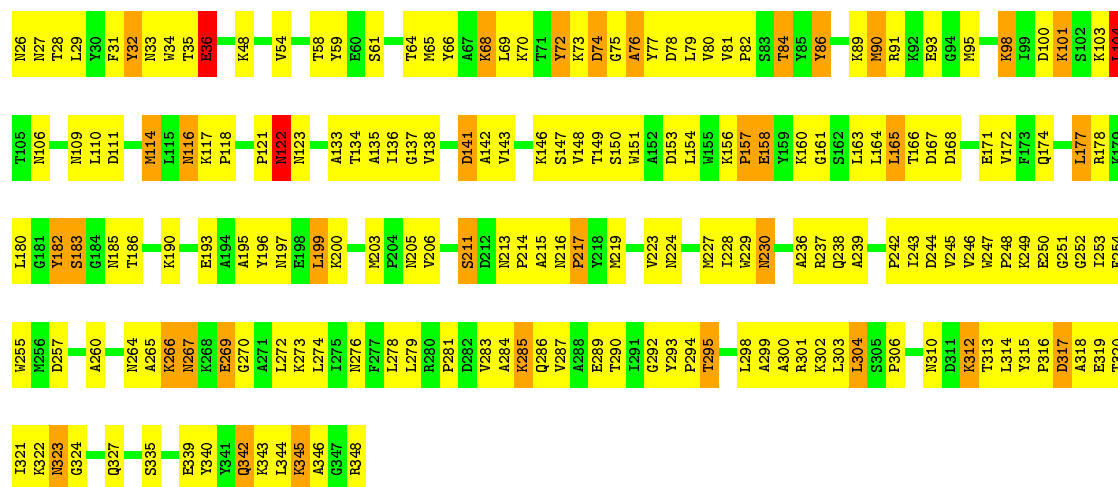


• Molecule 1: SPERMIDINE/PUTRESCINE-BINDING PROTEIN



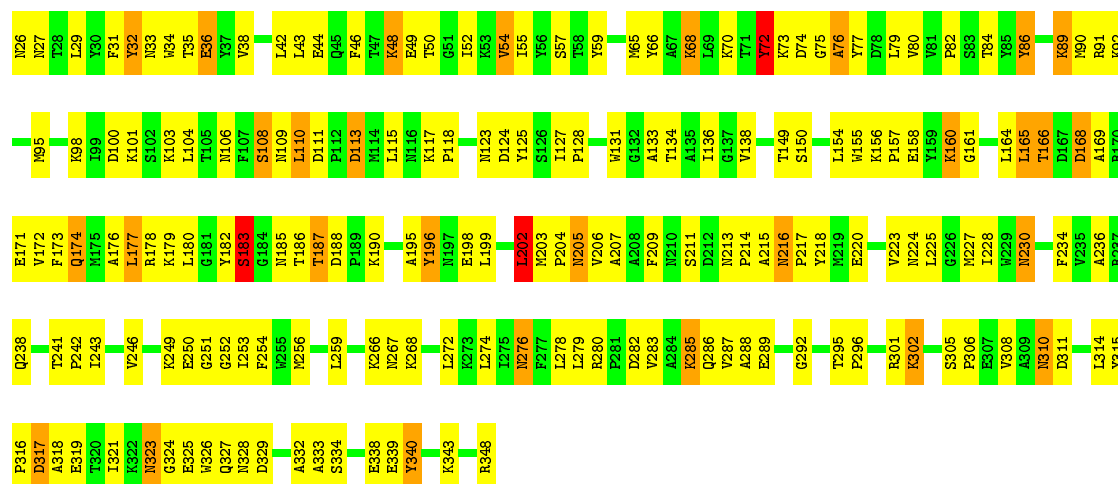
• Molecule 1: SPERMIDINE/PUTRESCINE-BINDING PROTEIN

Chain 3:  41% 48% 11%



- Molecule 1: SPERMIDINE/PUTRESCINE-BINDING PROTEIN

Chain 4: 43% 47% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.30Å 69.10Å 72.50Å 90.00° 107.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 71.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.50) 59.5 (71.01-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , 0.280 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	10.2	Xtriage
Anisotropy	1.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 55180 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10512	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 38.14 % 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 3.8549e-04.*

¹Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1	0.71	1/2623 (0.0%)	0.90	4/3568 (0.1%)
1	2	0.74	0/2626	0.92	5/3572 (0.1%)
1	3	0.76	1/2626 (0.0%)	0.90	3/3572 (0.1%)
1	4	0.76	0/2626	0.88	5/3572 (0.1%)
All	All	0.74	2/10501 (0.0%)	0.90	17/14284 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
1	3	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	76	ALA	CA-CB	-6.12	1.39	1.52
1	3	122	ASN	CA-CB	5.93	1.68	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	72	TYR	N-CA-C	8.16	133.04	111.00
1	4	202	LEU	CA-CB-CG	6.88	131.12	115.30
1	2	183	SER	N-CA-C	6.64	128.94	111.00
1	2	75	GLY	N-CA-C	-6.36	97.19	113.10
1	2	252	GLY	N-CA-C	-6.17	97.68	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	164	LEU	CA-CB-CG	6.11	129.36	115.30
1	4	251	GLY	N-CA-C	6.04	128.20	113.10
1	3	183	SER	N-CA-C	5.92	126.98	111.00
1	4	72	TYR	N-CA-C	5.83	126.74	111.00
1	2	163	LEU	CA-CB-CG	5.72	128.46	115.30
1	1	115	LEU	CA-CB-CG	5.70	128.42	115.30
1	4	115	LEU	CA-CB-CG	5.66	128.33	115.30
1	1	35	THR	N-CA-C	5.63	126.21	111.00
1	4	183	SER	N-CA-C	5.41	125.62	111.00
1	1	104	LEU	CA-CB-CG	5.39	127.70	115.30
1	3	252	GLY	N-CA-C	-5.19	100.14	113.10
1	3	104	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	30	TYR	Sidechain
1	3	182	TYR	Sidechain

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	1	2557	0	2502	185	0
1	2	2560	0	2504	177	0
1	3	2560	0	2504	189	0
1	4	2560	0	2504	147	0
2	1	10	0	19	8	0
2	2	10	0	19	10	0
2	3	10	0	19	5	0
2	4	10	0	19	5	0
3	1	59	0	0	3	0
3	2	53	0	0	11	0
3	3	71	0	0	12	0
3	4	52	0	0	5	0
All	All	10512	0	10090	694	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (694) 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)
1:3:32:TYR:HB2	1:3:76:ALA:HB3	1.30	1.07
1:1:73:LYS:HA	1:1:77:TYR:HE1	1.24	1.00
1:3:342:GLN:HA	1:3:342:GLN:HE21	1.27	0.95
1:2:160:LYS:HA	1:2:205:ASN:ND2	1.82	0.94
1:1:93:GLU:HB3	1:1:95:MET:HG3	1.49	0.93
1:1:36:GLU:HG3	2:1:400:SPD:N1	1.83	0.93
1:2:62:ASN:HD21	1:2:83:SER:HB2	1.34	0.93
1:2:266:LYS:HA	1:2:266:LYS:HE2	1.50	0.92
1:2:32:TYR:HB2	1:2:76:ALA:HB3	1.52	0.92
1:3:69:LEU:HD23	1:3:95:MET:HE2	1.52	0.91
1:4:73:LYS:HA	1:4:77:TYR:HE1	1.34	0.91
1:3:73:LYS:HA	1:3:77:TYR:HE1	1.35	0.89
1:4:318:ALA:HA	1:4:321:ILE:HG12	1.53	0.88
1:1:73:LYS:HA	1:1:77:TYR:CE1	2.08	0.88
1:3:317:ASP:HB2	1:3:320:THR:HG23	1.56	0.87
1:2:111:ASP:HB2	1:2:298:LEU:HD22	1.56	0.87
1:2:160:LYS:HA	1:2:205:ASN:HD22	1.39	0.86
1:3:66:TYR:CE1	1:3:70:LYS:HE3	2.10	0.86
1:4:150:SER:HB3	1:4:249:LYS:HE2	1.57	0.85
1:1:185:ASN:ND2	1:1:328:ASN:H	1.74	0.85
1:2:333:ALA:HB1	3:2:538:HOH:O	1.76	0.85
1:3:101:LYS:HZ3	1:3:104:LEU:HD23	1.41	0.84
1:3:32:TYR:HB2	1:3:76:ALA:CB	2.08	0.84
1:1:74:ASP:HB2	3:1:534:HOH:O	1.76	0.83
1:2:186:THR:HG22	1:2:188:ASP:H	1.43	0.83
1:2:110:LEU:HD21	1:2:279:LEU:HD22	1.58	0.83
1:4:106:ASN:H	1:4:276:ASN:HD21	1.22	0.83
1:1:164:LEU:HB2	1:1:223:VAL:HG21	1.60	0.83
1:3:106:ASN:H	1:3:276:ASN:HD21	1.28	0.81
1:1:180:LEU:HD13	1:1:182:TYR:CE2	2.14	0.81
1:1:168:ASP:O	1:1:172:VAL:HG23	1.81	0.80
1:2:150:SER:HB3	1:2:249:LYS:HE2	1.62	0.80
1:2:106:ASN:H	1:2:276:ASN:HD21	1.26	0.80
1:1:34:TRP:CH2	2:1:400:SPD:H71	2.18	0.79
1:3:157:PRO:O	1:3:160:LYS:HG3	1.83	0.79
1:3:158:GLU:HB3	3:3:582:HOH:O	1.82	0.78
1:1:32:TYR:HB2	1:1:76:ALA:CB	2.14	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:254:PHE:HE2	1:1:324:GLY:HA3	1.49	0.78
1:2:159:TYR:HB3	1:2:163:LEU:HD11	1.64	0.77
1:1:117:LYS:HB2	1:1:119:PHE:CE2	2.19	0.77
1:1:301:ARG:HA	1:1:304:LEU:HD22	1.66	0.77
1:4:168:ASP:O	1:4:172:VAL:HG23	1.83	0.77
1:1:185:ASN:HD22	1:1:328:ASN:HB2	1.49	0.77
1:4:160:LYS:H	1:4:160:LYS:HD3	1.48	0.77
1:1:111:ASP:HB2	1:1:298:LEU:HD22	1.63	0.77
1:2:86:TYR:O	1:2:90:MET:HG2	1.85	0.76
1:3:73:LYS:HA	1:3:77:TYR:CE1	2.20	0.76
1:4:266:LYS:HE2	1:4:266:LYS:HA	1.65	0.76
1:3:36:GLU:HG3	2:3:400:SPD:N1	2.01	0.76
1:1:36:GLU:HG3	2:1:400:SPD:HN12	1.50	0.76
1:1:118:PRO:O	1:1:121:PRO:HD3	1.86	0.75
1:4:138:VAL:HG12	1:4:225:LEU:HB2	1.68	0.75
1:1:185:ASN:ND2	1:1:328:ASN:HB2	2.02	0.75
1:2:36:GLU:HG3	2:2:400:SPD:HN12	1.51	0.75
1:3:68:LYS:HE3	1:3:72:TYR:CB	2.17	0.74
1:3:167:ASP:HB3	1:3:211:SER:HB2	1.69	0.74
1:1:32:TYR:HB2	1:1:76:ALA:HB1	1.70	0.73
1:4:36:GLU:HG2	2:4:400:SPD:N1	2.04	0.73
1:2:317:ASP:OD1	1:2:319:GLU:HB3	1.89	0.73
1:1:88:ASP:O	1:1:92:LYS:HG2	1.88	0.73
1:2:185:ASN:ND2	1:2:328:ASN:HB2	2.04	0.72
1:2:43:LEU:HG	1:2:54:VAL:HG11	1.72	0.72
1:2:166:THR:HB	1:2:227:MET:HE3	1.71	0.72
1:4:66:TYR:CE1	1:4:95:MET:SD	2.83	0.72
1:4:138:VAL:HG12	1:4:225:LEU:CB	2.20	0.72
1:1:100:ASP:OD1	1:1:103:LYS:HG2	1.89	0.72
1:1:254:PHE:CE2	1:1:324:GLY:HA3	2.25	0.71
1:3:203:MET:CE	1:3:348:ARG:HH12	2.02	0.71
1:3:68:LYS:HE3	1:3:72:TYR:CG	2.25	0.71
1:4:185:ASN:CG	1:4:328:ASN:HB2	2.10	0.71
1:1:185:ASN:HD22	1:1:328:ASN:H	1.36	0.71
1:1:318:ALA:HA	1:1:321:ILE:CD1	2.21	0.70
1:4:43:LEU:HD13	1:4:54:VAL:CG2	2.19	0.70
1:3:116:ASN:H	1:3:116:ASN:HD22	1.37	0.70
1:4:177:LEU:CD1	1:4:195:ALA:HB2	2.21	0.70
1:1:101:LYS:HZ2	1:1:107:PHE:HD2	1.39	0.70
1:1:316:PRO:HB2	1:1:320:THR:OG1	1.92	0.69
1:2:136:ILE:HB	1:2:246:VAL:HG22	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:157:PRO:O	1:2:160:LYS:HE2	1.93	0.69
1:4:213:ASN:ND2	1:4:216:ASN:HD22	1.88	0.69
1:3:190:LYS:O	1:3:193:GLU:HB3	1.92	0.69
1:2:117:LYS:HD2	1:2:117:LYS:N	2.06	0.69
1:2:66:TYR:CE1	1:2:95:MET:SD	2.85	0.69
1:1:318:ALA:HA	1:1:321:ILE:HD11	1.75	0.69
1:2:318:ALA:HA	1:2:321:ILE:HG12	1.73	0.69
1:1:136:ILE:HB	1:1:246:VAL:HG22	1.75	0.69
1:1:26:ASN:HB3	3:1:634:HOH:O	1.92	0.69
1:4:314:LEU:O	1:4:316:PRO:HD3	1.91	0.69
1:4:73:LYS:HA	1:4:77:TYR:CE1	2.24	0.69
1:1:166:THR:HG21	1:1:171:GLU:OE1	1.92	0.69
1:4:228:ILE:HD13	1:4:243:ILE:HD11	1.75	0.69
1:4:230:ASN:N	1:4:230:ASN:HD22	1.91	0.68
1:2:281:PRO:O	1:2:285:LYS:HB2	1.91	0.68
1:3:312:LYS:HG2	1:3:313:THR:N	2.07	0.68
1:1:177:LEU:HB3	1:1:183:SER:HB3	1.75	0.68
1:3:237:ARG:HD2	1:3:243:ILE:O	1.93	0.68
1:1:117:LYS:HD2	1:1:117:LYS:N	2.08	0.68
1:1:101:LYS:HE3	1:1:127:ILE:HD11	1.75	0.68
1:3:168:ASP:HB3	1:3:171:GLU:HB2	1.75	0.68
1:2:268:LYS:HB3	1:2:268:LYS:NZ	2.09	0.68
1:2:32:TYR:HB2	1:2:76:ALA:CB	2.22	0.67
1:3:70:LYS:HB2	1:3:70:LYS:HZ2	1.59	0.67
1:3:100:ASP:OD2	1:3:103:LYS:HG2	1.94	0.67
1:2:214:PRO:O	1:2:217:PRO:HD2	1.95	0.67
1:2:166:THR:HB	1:2:227:MET:CE	2.24	0.67
1:2:34:TRP:CZ3	2:2:400:SPD:H71	2.29	0.67
1:3:199:LEU:HG	1:3:344:LEU:HD21	1.77	0.67
1:1:228:ILE:HD13	1:1:233:ALA:HB2	1.78	0.66
1:2:38:VAL:HB	1:2:42:LEU:HD23	1.77	0.66
1:2:65:MET:SD	1:2:80:VAL:HG11	2.34	0.66
1:4:36:GLU:HG2	2:4:400:SPD:HN12	1.60	0.66
1:3:245:VAL:HB	1:3:313:THR:HG22	1.76	0.66
1:2:301:ARG:HA	1:2:304:LEU:HD22	1.76	0.66
1:4:86:TYR:O	1:4:90:MET:HG2	1.96	0.66
1:3:216:ASN:HB3	1:3:217:PRO:HD3	1.78	0.66
1:2:37:TYR:CZ	2:2:400:SPD:H41	2.31	0.66
1:3:178:ARG:HG2	1:3:183:SER:HB2	1.77	0.65
1:4:180:LEU:HD12	1:4:180:LEU:N	2.11	0.65
1:2:165:LEU:HD13	1:2:206:VAL:HG22	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:86:TYR:O	1:1:90:MET:HG2	1.97	0.65
1:2:268:LYS:O	1:2:272:LEU:HD23	1.97	0.65
1:4:32:TYR:HB2	1:4:76:ALA:CB	2.27	0.65
1:2:100:ASP:OD2	1:2:103:LYS:HG2	1.97	0.65
1:3:160:LYS:HD3	3:3:551:HOH:O	1.96	0.64
1:4:33:ASN:ND2	1:4:34:TRP:H	1.94	0.64
1:3:78:ASP:HA	1:3:265:ALA:HB1	1.79	0.64
1:3:70:LYS:HB2	1:3:70:LYS:NZ	2.12	0.64
1:4:32:TYR:HB2	1:4:76:ALA:HB3	1.78	0.64
1:2:266:LYS:CA	1:2:266:LYS:HE2	2.25	0.64
1:1:117:LYS:H	1:1:117:LYS:HD2	1.63	0.64
1:1:185:ASN:ND2	1:1:328:ASN:N	2.46	0.64
1:2:241:THR:HG23	3:2:639:HOH:O	1.96	0.64
1:3:284:ALA:HB1	1:3:295:THR:HG21	1.80	0.64
1:1:177:LEU:HB3	1:1:183:SER:HA	1.80	0.64
1:3:203:MET:HE1	1:3:348:ARG:HH12	1.62	0.64
1:3:197:ASN:O	1:3:200:LYS:HB2	1.98	0.64
1:1:177:LEU:HB3	1:1:183:SER:CB	2.28	0.63
1:2:165:LEU:HA	1:2:227:MET:HG3	1.79	0.63
1:2:138:VAL:O	1:2:243:ILE:HA	1.98	0.63
1:3:151:TRP:HA	1:3:154:LEU:HD13	1.80	0.63
1:1:97:GLN:HB3	1:1:263:ALA:HA	1.79	0.63
1:4:306:PRO:O	1:4:310:ASN:HB3	1.97	0.63
1:3:213:ASN:ND2	1:3:216:ASN:HD22	1.97	0.63
1:1:319:GLU:O	1:1:322:LYS:HE2	1.97	0.63
1:3:317:ASP:HB3	1:3:319:GLU:H	1.64	0.63
1:2:159:TYR:HB3	1:2:163:LEU:CD1	2.28	0.62
1:2:126:SER:O	1:2:127:ILE:HD13	1.98	0.62
1:1:80:VAL:HG12	1:1:82:PRO:HD3	1.81	0.62
1:2:166:THR:HG22	1:2:168:ASP:HB2	1.80	0.62
1:2:73:LYS:HA	1:2:77:TYR:CE1	2.34	0.62
1:3:29:LEU:HD23	1:3:274:LEU:HD22	1.82	0.62
1:2:176:ALA:O	1:2:180:LEU:HD12	2.00	0.62
1:1:139:ASN:OD1	1:1:141:ASP:HB3	1.99	0.62
1:4:59:TYR:CE2	1:4:65:MET:HG3	2.35	0.62
1:2:32:TYR:CB	1:2:76:ALA:HB3	2.26	0.62
1:4:318:ALA:HA	1:4:321:ILE:CG1	2.27	0.62
1:1:155:TRP:NE1	1:1:202:LEU:HB2	2.15	0.62
1:3:213:ASN:HD22	1:3:216:ASN:HD22	1.48	0.62
1:3:180:LEU:HD13	1:3:182:TYR:CE1	2.35	0.62
1:1:117:LYS:H	1:1:117:LYS:CD	2.12	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:43:LEU:HD13	1:4:54:VAL:HG21	1.81	0.62
1:1:247:TRP:CZ2	1:1:316:PRO:HB3	2.34	0.61
1:3:36:GLU:HG3	2:3:400:SPD:HN12	1.62	0.61
1:3:91:ARG:HG2	1:3:91:ARG:NH1	2.14	0.61
1:1:177:LEU:HB3	1:1:183:SER:CA	2.30	0.61
1:4:43:LEU:HD13	1:4:54:VAL:HG22	1.82	0.61
1:3:348:ARG:HB2	1:3:348:ARG:NH1	2.15	0.61
1:3:150:SER:HB3	1:3:249:LYS:HB3	1.82	0.61
1:2:254:PHE:CZ	1:2:321:ILE:HG22	2.36	0.61
1:3:101:LYS:HA	1:3:104:LEU:HD23	1.83	0.61
1:4:177:LEU:HD13	1:4:195:ALA:HB2	1.83	0.61
1:3:317:ASP:HB3	1:3:319:GLU:HB3	1.81	0.60
1:3:299:ALA:O	1:3:303:LEU:HD13	2.01	0.60
1:3:215:ALA:HB2	1:3:228:ILE:HD11	1.82	0.60
1:2:182:TYR:O	1:2:183:SER:HB3	2.02	0.60
1:2:106:ASN:HB2	1:2:276:ASN:ND2	2.15	0.60
1:1:199:LEU:O	1:1:203:MET:HG2	2.01	0.60
1:1:68:LYS:HA	1:1:68:LYS:CE	2.32	0.60
1:2:33:ASN:O	1:2:58:THR:HA	2.01	0.60
1:3:142:ALA:HB2	3:4:573:HOH:O	2.00	0.60
1:2:299:ALA:O	1:2:303:LEU:HD22	2.02	0.60
1:4:327:GLN:OE1	2:4:400:SPD:N10	2.34	0.60
1:2:312:LYS:O	1:2:312:LYS:HG2	2.01	0.60
1:4:131:TRP:HA	1:4:256:MET:HA	1.82	0.60
1:3:136:ILE:HD11	1:3:248:PRO:HB3	1.84	0.60
1:4:72:TYR:HD1	1:4:74:ASP:H	1.49	0.60
1:3:196:TYR:O	1:3:200:LYS:HG3	2.03	0.59
1:3:117:LYS:N	1:3:117:LYS:HD2	2.16	0.59
1:3:317:ASP:O	1:3:321:ILE:HG23	2.01	0.59
1:2:213:ASN:ND2	1:2:216:ASN:ND2	2.50	0.59
1:3:153:ASP:O	1:3:156:LYS:HG3	2.03	0.59
1:1:173:PHE:O	1:1:177:LEU:HD22	2.03	0.59
1:1:319:GLU:O	1:1:322:LYS:HB3	2.02	0.59
1:3:178:ARG:HG2	1:3:183:SER:CB	2.32	0.59
1:2:186:THR:HG22	1:2:187:THR:N	2.18	0.59
1:1:269:GLU:HA	1:1:272:LEU:HD23	1.84	0.59
1:2:37:TYR:OH	2:2:400:SPD:H41	2.03	0.58
1:3:86:TYR:O	1:3:90:MET:HG2	2.02	0.58
1:1:180:LEU:HD13	1:1:182:TYR:CD2	2.37	0.58
1:2:241:THR:O	1:2:243:ILE:HG22	2.03	0.58
1:2:36:GLU:HG3	2:2:400:SPD:N1	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:228:ILE:HD12	1:1:243:ILE:HD11	1.86	0.58
1:1:185:ASN:OD1	1:1:185:ASN:N	2.36	0.58
1:2:186:THR:HG22	1:2:188:ASP:N	2.16	0.58
1:1:254:PHE:CE2	1:1:321:ILE:HA	2.39	0.58
1:1:157:PRO:O	1:1:160:LYS:HG3	2.03	0.58
1:2:284:ALA:O	1:2:287:VAL:HG12	2.03	0.58
1:1:285:LYS:HD2	1:1:303:LEU:HB3	1.83	0.58
1:3:230:ASN:HD22	1:3:230:ASN:N	2.00	0.58
1:1:177:LEU:C	1:1:183:SER:HB3	2.25	0.58
1:1:301:ARG:HG2	1:1:301:ARG:HH11	1.69	0.58
1:1:230:ASN:HD22	1:1:230:ASN:N	2.02	0.58
1:3:91:ARG:HH11	1:3:91:ARG:HG2	1.68	0.57
1:1:33:ASN:ND2	1:1:34:TRP:H	2.03	0.57
1:2:31:PHE:HD1	1:2:79:LEU:HB3	1.69	0.57
1:1:176:ALA:O	1:1:179:LYS:HB3	2.04	0.57
1:1:185:ASN:HD22	1:1:328:ASN:N	1.98	0.57
1:4:46:PHE:CE1	1:4:50:THR:HG21	2.39	0.57
1:4:178:ARG:HH12	1:4:324:GLY:C	2.07	0.57
1:3:101:LYS:NZ	1:3:104:LEU:HD23	2.16	0.57
1:3:31:PHE:CE1	1:3:33:ASN:HB2	2.39	0.57
1:3:270:GLY:O	1:3:273:LYS:HB2	2.05	0.57
1:1:68:LYS:NZ	1:1:68:LYS:HA	2.19	0.57
1:2:186:THR:HG22	1:2:187:THR:H	1.70	0.57
1:3:116:ASN:ND2	1:3:116:ASN:H	2.02	0.57
1:4:287:VAL:HG13	1:4:288:ALA:N	2.19	0.57
1:4:36:GLU:CG	2:4:400:SPD:N1	2.67	0.57
1:2:228:ILE:HD13	1:2:243:ILE:HD11	1.85	0.57
1:3:32:TYR:HB3	1:3:80:VAL:HG13	1.87	0.56
1:4:234:PHE:CD2	1:4:292:GLY:HA3	2.39	0.56
1:2:135:ALA:HB3	1:2:245:VAL:HG13	1.85	0.56
1:3:84:THR:HB	3:3:717:HOH:O	2.04	0.56
1:4:254:PHE:CE2	1:4:324:GLY:HA3	2.40	0.56
1:4:164:LEU:HD21	1:4:217:PRO:HG2	1.86	0.56
1:3:348:ARG:HH11	1:3:348:ARG:HB2	1.70	0.56
1:3:166:THR:HG21	1:3:171:GLU:OE1	2.04	0.56
1:3:59:TYR:CE2	1:3:65:MET:HG3	2.41	0.56
1:4:66:TYR:CE2	1:4:70:LYS:HE3	2.41	0.56
1:1:318:ALA:HA	1:1:321:ILE:HG12	1.88	0.56
1:4:79:LEU:HD21	1:4:259:LEU:HD22	1.87	0.56
1:1:91:ARG:HD2	1:1:125:TYR:CE2	2.41	0.56
1:3:33:ASN:ND2	1:3:81:VAL:HG21	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:342:GLN:HB3	3:3:666:HOH:O	2.06	0.55
1:4:29:LEU:HD21	1:4:274:LEU:HD22	1.87	0.55
1:2:73:LYS:HG3	1:2:74:ASP:N	2.21	0.55
1:3:269:GLU:O	1:3:273:LYS:HG3	2.06	0.55
1:2:111:ASP:CB	1:2:298:LEU:HD22	2.34	0.55
1:4:90:MET:HB2	1:4:95:MET:HB2	1.89	0.55
1:3:29:LEU:CD2	1:3:274:LEU:HD22	2.36	0.55
1:2:166:THR:CG2	1:2:168:ASP:HB2	2.36	0.55
1:1:192:ILE:O	1:1:195:ALA:HB3	2.07	0.55
1:4:66:TYR:CZ	1:4:89:LYS:HE2	2.41	0.55
1:4:328:ASN:HA	3:4:663:HOH:O	2.06	0.55
1:3:292:GLY:O	1:3:314:LEU:HD22	2.05	0.55
1:3:323:ASN:HD22	1:3:324:GLY:N	2.04	0.55
1:1:48:LYS:HA	1:1:48:LYS:NZ	2.22	0.55
1:1:318:ALA:HA	1:1:321:ILE:CG1	2.37	0.55
1:4:166:THR:HG21	1:4:171:GLU:OE1	2.06	0.55
1:1:186:THR:HG22	1:1:188:ASP:H	1.71	0.55
1:2:77:TYR:O	1:2:262:PRO:HG2	2.07	0.55
1:1:110:LEU:HA	1:1:297:ASN:HA	1.89	0.55
1:3:133:ALA:HB2	1:3:254:PHE:CD1	2.42	0.54
1:1:185:ASN:HD22	1:1:328:ASN:CB	2.19	0.54
1:1:285:LYS:HB2	1:1:300:ALA:HB1	1.89	0.54
1:1:117:LYS:HB2	1:1:119:PHE:CD2	2.42	0.54
1:3:295:THR:HG23	3:3:729:HOH:O	2.05	0.54
1:4:178:ARG:HG2	1:4:183:SER:CB	2.37	0.54
1:1:117:LYS:CB	1:1:119:PHE:CE2	2.90	0.54
1:1:202:LEU:O	1:1:202:LEU:HG	2.07	0.54
1:1:161:GLY:H	1:1:205:ASN:HA	1.72	0.54
1:3:165:LEU:HA	1:3:227:MET:HG2	1.89	0.54
1:4:32:TYR:CG	1:4:76:ALA:HB3	2.43	0.54
1:1:348:ARG:HH11	1:1:348:ARG:HB3	1.73	0.54
1:3:98:LYS:H	1:3:98:LYS:HD3	1.73	0.54
1:3:283:VAL:O	1:3:286:GLN:HB3	2.06	0.54
1:3:164:LEU:HB2	1:3:223:VAL:HG21	1.89	0.54
1:2:173:PHE:HZ	1:2:340:TYR:HB3	1.73	0.54
1:3:342:GLN:HA	1:3:342:GLN:NE2	2.09	0.54
1:1:36:GLU:HG3	2:1:400:SPD:HN11	1.69	0.54
1:3:150:SER:HB3	1:3:249:LYS:CB	2.38	0.54
1:2:180:LEU:HD23	1:2:182:TYR:CE1	2.42	0.54
1:4:164:LEU:HB2	1:4:223:VAL:HG21	1.90	0.54
1:3:327:GLN:OE1	2:3:400:SPD:N10	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:66:TYR:HE1	1:4:95:MET:SD	2.30	0.53
1:1:36:GLU:CG	2:1:400:SPD:HN12	2.20	0.53
1:3:77:TYR:CB	3:3:564:HOH:O	2.56	0.53
1:2:192:ILE:HD12	3:2:538:HOH:O	2.07	0.53
1:1:52:ILE:HD11	1:1:273:LYS:HD2	1.90	0.53
1:2:180:LEU:HB3	1:2:182:TYR:HD1	1.73	0.53
1:3:136:ILE:HB	1:3:246:VAL:HG23	1.91	0.53
1:2:134:THR:HB	1:2:253:ILE:HB	1.91	0.53
1:2:62:ASN:ND2	1:2:83:SER:HB2	2.13	0.53
1:3:81:VAL:HG12	1:3:257:ASP:HB3	1.91	0.53
1:3:320:THR:O	1:3:323:ASN:ND2	2.42	0.53
1:2:139:ASN:HA	1:2:242:PRO:O	2.09	0.53
1:2:91:ARG:HD2	1:2:125:TYR:CE1	2.43	0.53
1:4:302:LYS:NZ	1:4:302:LYS:HB3	2.24	0.53
1:2:192:ILE:CD1	3:2:538:HOH:O	2.57	0.53
1:4:280:ARG:HB3	1:4:282:ASP:OD1	2.08	0.53
1:1:42:LEU:HD11	1:1:277:PHE:HE2	1.74	0.53
1:3:342:GLN:CA	1:3:342:GLN:HE21	2.08	0.53
1:1:214:PRO:HG2	1:1:229:TRP:CE3	2.44	0.53
1:1:180:LEU:HD12	1:1:180:LEU:C	2.28	0.53
1:2:98:LYS:HD2	1:2:125:TYR:OH	2.09	0.53
1:2:251:GLY:HA2	1:2:323:ASN:O	2.08	0.53
1:2:171:GLU:OE2	2:2:400:SPD:N10	2.42	0.53
1:3:61:SER:HB3	1:3:64:THR:OG1	2.09	0.53
1:4:168:ASP:HB3	1:4:171:GLU:HB2	1.91	0.53
1:1:342:GLN:HA	1:1:342:GLN:NE2	2.22	0.53
1:2:65:MET:SD	1:2:80:VAL:CG1	2.96	0.52
1:3:317:ASP:CB	1:3:319:GLU:HB3	2.39	0.52
1:3:70:LYS:CB	1:3:70:LYS:NZ	2.71	0.52
1:1:101:LYS:CE	1:1:127:ILE:HD11	2.39	0.52
1:1:106:ASN:HB3	1:1:109:ASN:ND2	2.24	0.52
1:2:69:LEU:HB3	1:2:95:MET:HE2	1.92	0.52
1:2:110:LEU:HD21	1:2:279:LEU:CD2	2.32	0.52
1:3:122:ASN:N	1:3:122:ASN:HD22	2.08	0.52
1:4:215:ALA:HB1	1:4:236:ALA:HB2	1.90	0.52
1:1:203:MET:HA	1:1:206:VAL:HG23	1.92	0.52
1:3:161:GLY:H	1:3:205:ASN:HA	1.75	0.52
1:3:285:LYS:O	1:3:289:GLU:HG3	2.08	0.52
1:3:33:ASN:ND2	1:3:34:TRP:H	2.07	0.52
1:3:174:GLN:O	1:3:178:ARG:HG3	2.10	0.52
1:3:81:VAL:CG1	1:3:257:ASP:HB3	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:68:LYS:HG2	1:4:75:GLY:HA3	1.91	0.52
1:4:110:LEU:HD21	1:4:279:LEU:HD21	1.91	0.52
1:4:178:ARG:HG2	1:4:183:SER:HB2	1.91	0.52
1:4:254:PHE:O	1:4:326:TRP:HA	2.09	0.52
1:1:254:PHE:O	1:1:326:TRP:HA	2.09	0.52
1:3:206:VAL:HB	1:3:348:ARG:NH2	2.25	0.52
1:1:44:GLU:O	1:1:48:LYS:HD2	2.10	0.52
1:2:213:ASN:ND2	1:2:216:ASN:HD22	2.08	0.51
1:1:106:ASN:H	1:1:276:ASN:HD21	1.55	0.51
1:3:318:ALA:O	1:3:322:LYS:HB2	2.09	0.51
1:2:311:ASP:OD2	1:2:314:LEU:HG	2.09	0.51
1:2:66:TYR:HE1	1:2:90:MET:HB3	1.75	0.51
1:3:319:GLU:HG2	1:3:320:THR:N	2.25	0.51
1:3:301:ARG:HA	1:3:304:LEU:HD22	1.93	0.51
1:2:241:THR:O	1:2:243:ILE:N	2.44	0.51
1:1:137:GLY:O	1:1:225:LEU:HA	2.10	0.51
1:3:285:LYS:HG2	1:3:285:LYS:O	2.11	0.51
1:4:155:TRP:CZ3	1:4:179:LYS:HD2	2.46	0.51
1:3:316:PRO:HB2	1:3:320:THR:OG1	2.10	0.51
1:1:180:LEU:CD1	1:1:182:TYR:CD2	2.94	0.51
1:2:151:TRP:O	1:2:154:LEU:HB2	2.10	0.51
1:1:52:ILE:CD1	1:1:273:LYS:HD2	2.40	0.51
1:4:254:PHE:CE2	1:4:321:ILE:HA	2.46	0.51
1:3:317:ASP:HB3	1:3:319:GLU:N	2.26	0.51
1:2:177:LEU:O	1:2:180:LEU:HB2	2.10	0.51
1:2:188:ASP:OD2	1:2:191:GLU:HG3	2.11	0.51
1:1:287:VAL:HG13	1:1:288:ALA:N	2.26	0.51
1:2:35:THR:HG21	1:2:212:ASP:OD1	2.11	0.51
1:1:255:TRP:CH2	2:1:400:SPD:H52	2.46	0.51
1:3:75:GLY:O	1:3:76:ALA:HB2	2.11	0.50
1:1:178:ARG:CZ	1:1:250:GLU:O	2.58	0.50
1:4:266:LYS:CA	1:4:266:LYS:HE2	2.36	0.50
1:2:80:VAL:HG12	1:2:81:VAL:N	2.26	0.50
1:1:122:ASN:OD1	1:1:124:ASP:OD2	2.29	0.50
1:2:81:VAL:CG1	1:2:257:ASP:HB3	2.42	0.50
1:4:195:ALA:O	1:4:199:LEU:HD23	2.11	0.50
1:2:164:LEU:HD21	1:2:210:ASN:HB2	1.93	0.50
1:1:133:ALA:HB2	1:1:254:PHE:HD1	1.77	0.50
1:3:294:PRO:HB3	1:3:315:TYR:CE1	2.46	0.50
1:1:111:ASP:OD1	1:1:113:ASP:HB2	2.10	0.50
1:1:138:VAL:HG12	1:1:225:LEU:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:27:ASN:CG	1:2:28:THR:H	2.15	0.50
1:4:174:GLN:OE1	1:4:325:GLU:HB3	2.11	0.50
1:3:136:ILE:HB	1:3:246:VAL:CG2	2.42	0.50
1:2:269:GLU:HA	3:2:632:HOH:O	2.10	0.50
1:4:138:VAL:HG12	1:4:225:LEU:HB3	1.94	0.49
1:3:172:VAL:HG12	1:3:199:LEU:HD21	1.94	0.49
1:2:177:LEU:HD23	1:2:184:GLY:N	2.27	0.49
1:1:301:ARG:O	1:1:304:LEU:HB2	2.12	0.49
1:1:137:GLY:HA2	1:1:244:ASP:O	2.12	0.49
1:3:77:TYR:HB2	3:3:565:HOH:O	2.11	0.49
1:3:149:THR:O	1:3:249:LYS:HB2	2.12	0.49
1:2:177:LEU:HG	1:2:183:SER:HA	1.94	0.49
1:1:318:ALA:O	1:1:321:ILE:HG12	2.12	0.49
1:4:31:PHE:CD1	1:4:79:LEU:HB3	2.48	0.49
1:3:121:PRO:HB2	1:3:122:ASN:HD22	1.76	0.49
1:1:33:ASN:HB3	1:1:56:TYR:OH	2.13	0.49
1:2:59:TYR:CZ	1:2:65:MET:HG3	2.48	0.49
1:1:177:LEU:HD13	1:1:195:ALA:HB2	1.95	0.49
1:4:285:LYS:HG3	1:4:286:GLN:N	2.27	0.49
1:1:100:ASP:CG	1:1:103:LYS:HG2	2.33	0.49
1:3:143:VAL:CG2	1:3:224:ASN:HB3	2.43	0.49
1:2:32:TYR:CG	1:2:76:ALA:HB3	2.48	0.49
1:2:178:ARG:HG2	1:2:183:SER:HB2	1.94	0.49
1:4:29:LEU:CD2	1:4:274:LEU:HD22	2.42	0.49
1:4:230:ASN:N	1:4:230:ASN:ND2	2.60	0.49
1:3:335:SER:O	1:3:339:GLU:HB2	2.12	0.49
1:2:33:ASN:ND2	1:2:81:VAL:HG21	2.27	0.49
1:3:101:LYS:HA	1:3:101:LYS:HZ2	1.77	0.49
1:3:245:VAL:HB	1:3:313:THR:CG2	2.42	0.49
1:1:186:THR:HG21	1:1:191:GLU:HB2	1.94	0.49
1:2:156:LYS:HB2	1:2:159:TYR:CE2	2.48	0.49
1:2:88:ASP:O	1:2:92:LYS:HG2	2.13	0.49
1:3:65:MET:O	1:3:69:LEU:HB2	2.12	0.49
1:3:101:LYS:HA	1:3:101:LYS:NZ	2.28	0.49
1:1:178:ARG:HG2	1:1:183:SER:HB2	1.94	0.49
1:4:100:ASP:OD2	1:4:103:LYS:HG2	2.13	0.49
1:2:34:TRP:CH2	2:2:400:SPD:H71	2.48	0.48
1:3:69:LEU:HD23	1:3:95:MET:CE	2.36	0.48
1:2:98:LYS:HG3	1:2:125:TYR:CZ	2.48	0.48
1:2:89:LYS:HA	1:2:92:LYS:NZ	2.28	0.48
1:4:339:GLU:O	1:4:343:LYS:HG3	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:241:THR:HA	1:4:242:PRO:HD3	1.64	0.48
1:4:292:GLY:O	1:4:314:LEU:HD13	2.13	0.48
1:2:268:LYS:HZ3	1:2:268:LYS:HB3	1.78	0.48
1:2:72:TYR:HE1	1:2:74:ASP:OD1	1.96	0.48
1:3:281:PRO:HA	1:3:300:ALA:HB2	1.95	0.48
1:4:38:VAL:HG23	1:4:38:VAL:O	2.13	0.48
1:4:169:ALA:O	1:4:173:PHE:HD2	1.96	0.48
1:4:215:ALA:O	1:4:218:TYR:HB2	2.13	0.48
1:3:343:LYS:O	1:3:346:ALA:HB3	2.13	0.48
1:3:34:TRP:HB3	2:3:400:SPD:H21	1.95	0.48
1:1:91:ARG:HD2	1:1:125:TYR:CD2	2.48	0.48
1:1:189:PRO:HB3	1:1:336:ILE:HD13	1.95	0.48
1:3:242:PRO:HD3	1:4:55:ILE:HG23	1.95	0.48
1:2:99:ILE:HA	3:2:635:HOH:O	2.13	0.48
1:1:58:THR:O	1:2:220:GLU:HA	2.14	0.48
1:4:136:ILE:HB	1:4:246:VAL:HG22	1.96	0.48
1:1:34:TRP:CZ3	2:1:400:SPD:H71	2.49	0.48
1:1:216:ASN:HB3	1:1:217:PRO:HD3	1.96	0.48
1:1:269:GLU:O	1:1:272:LEU:HB2	2.14	0.48
1:3:178:ARG:NH1	1:3:251:GLY:HA3	2.29	0.48
1:3:323:ASN:ND2	1:3:323:ASN:C	2.68	0.48
1:1:111:ASP:OD2	1:1:114:MET:HG2	2.13	0.48
1:2:261:ILE:HG21	1:2:268:LYS:HG3	1.95	0.48
1:4:106:ASN:HB2	1:4:276:ASN:ND2	2.29	0.47
1:1:186:THR:HG22	1:1:188:ASP:N	2.29	0.47
1:4:214:PRO:HB2	1:4:228:ILE:HG13	1.95	0.47
1:2:31:PHE:CD1	1:2:79:LEU:HB3	2.48	0.47
1:1:182:TYR:CD2	1:1:191:GLU:HG2	2.48	0.47
1:4:199:LEU:O	1:4:203:MET:HG2	2.13	0.47
1:3:143:VAL:HG23	1:3:224:ASN:HB3	1.96	0.47
1:3:137:GLY:HA2	1:3:244:ASP:O	2.15	0.47
1:2:34:TRP:CD1	1:2:34:TRP:N	2.82	0.47
1:3:68:LYS:HE3	1:3:72:TYR:HB2	1.95	0.47
1:1:103:LYS:HB3	1:1:103:LYS:HE2	1.73	0.47
1:2:148:VAL:HG11	1:2:225:LEU:HD12	1.95	0.47
1:3:177:LEU:HD13	1:3:195:ALA:HB2	1.96	0.47
1:3:100:ASP:O	1:3:104:LEU:HD22	2.13	0.47
1:3:174:GLN:OE1	1:3:253:ILE:HG23	2.14	0.47
1:4:203:MET:N	1:4:204:PRO:HD2	2.29	0.47
1:4:243:ILE:O	1:4:243:ILE:HG23	2.14	0.47
1:1:243:ILE:O	1:1:243:ILE:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:267:ASN:ND2	1:3:270:GLY:H	2.12	0.47
1:1:28:THR:HA	1:1:53:LYS:O	2.14	0.47
1:4:80:VAL:HG12	1:4:82:PRO:HD3	1.96	0.47
1:2:69:LEU:HD11	1:2:80:VAL:HG21	1.96	0.47
1:1:101:LYS:HZ3	1:1:101:LYS:HA	1.79	0.47
1:1:90:MET:HB2	1:1:95:MET:HB2	1.95	0.47
1:3:77:TYR:O	1:3:265:ALA:HA	2.15	0.47
1:1:283:VAL:O	1:1:287:VAL:HG12	2.14	0.47
1:3:106:ASN:HB3	1:3:279:LEU:HB3	1.97	0.47
1:3:203:MET:HE3	1:3:348:ARG:HH12	1.77	0.47
1:4:44:GLU:O	1:4:48:LYS:HD2	2.14	0.47
1:1:151:TRP:CZ2	1:1:248:PRO:HG3	2.50	0.47
1:3:255:TRP:CH2	2:3:400:SPD:H52	2.50	0.46
1:4:27:ASN:N	1:4:27:ASN:OD1	2.48	0.46
1:4:186:THR:HG22	1:4:187:THR:N	2.30	0.46
1:1:36:GLU:CG	2:1:400:SPD:N1	2.67	0.46
1:3:254:PHE:CE2	1:3:321:ILE:HA	2.51	0.46
1:1:304:LEU:HB3	1:1:309:ALA:HB2	1.98	0.46
1:2:43:LEU:HG	1:2:54:VAL:CG1	2.44	0.46
1:3:313:THR:HB	3:3:716:HOH:O	2.15	0.46
1:4:196:TYR:CD2	1:4:340:TYR:CD1	3.03	0.46
1:3:82:PRO:HB3	1:3:90:MET:SD	2.55	0.46
1:3:110:LEU:HD21	1:3:279:LEU:HD22	1.97	0.46
1:2:118:PRO:O	1:2:121:PRO:HD3	2.15	0.46
1:2:174:GLN:HE21	1:2:174:GLN:HB2	1.59	0.46
1:1:33:ASN:ND2	1:1:81:VAL:HG21	2.31	0.46
1:1:87:VAL:O	1:1:91:ARG:HB2	2.15	0.46
1:1:150:SER:HB2	1:1:250:GLU:OE1	2.15	0.46
1:2:151:TRP:CE2	1:2:248:PRO:HG3	2.50	0.46
1:4:180:LEU:CD1	1:4:180:LEU:N	2.78	0.46
1:3:151:TRP:O	1:3:154:LEU:HB2	2.15	0.46
1:3:58:THR:O	1:4:220:GLU:HA	2.16	0.46
1:3:151:TRP:O	1:3:154:LEU:HD13	2.16	0.46
1:4:49:GLU:OE2	1:4:280:ARG:NH2	2.48	0.46
1:4:323:ASN:ND2	1:4:323:ASN:O	2.49	0.46
1:1:177:LEU:CD1	1:1:195:ALA:HB2	2.46	0.45
1:1:26:ASN:CB	3:1:634:HOH:O	2.57	0.45
1:4:32:TYR:CB	1:4:76:ALA:HB3	2.44	0.45
1:1:173:PHE:CD1	1:1:195:ALA:HB1	2.50	0.45
1:1:165:LEU:O	1:1:209:PHE:HA	2.15	0.45
1:4:117:LYS:HA	1:4:118:PRO:HD3	1.88	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:271:ALA:O	1:1:275:ILE:HG13	2.16	0.45
1:1:281:PRO:HG3	1:1:299:ALA:HB3	1.98	0.45
1:2:196:TYR:OH	1:2:200:LYS:NZ	2.49	0.45
1:2:182:TYR:O	1:2:183:SER:CB	2.62	0.45
1:1:304:LEU:HD12	1:1:304:LEU:HA	1.77	0.45
1:3:167:ASP:OD1	1:3:345:LYS:HE3	2.15	0.45
1:2:272:LEU:HB2	3:2:632:HOH:O	2.17	0.45
1:3:249:LYS:HE2	1:3:249:LYS:HB2	1.76	0.45
1:1:181:GLY:O	1:1:182:TYR:C	2.54	0.45
1:3:134:THR:HG21	1:3:227:MET:HE2	1.98	0.45
1:3:77:TYR:HB2	3:3:564:HOH:O	2.15	0.45
1:2:180:LEU:HB3	1:2:182:TYR:CD1	2.51	0.45
1:2:110:LEU:CD2	1:2:279:LEU:HD22	2.37	0.45
1:3:110:LEU:HD21	1:3:279:LEU:CD2	2.46	0.45
1:3:78:ASP:HA	1:3:265:ALA:CB	2.46	0.45
1:2:249:LYS:HG2	1:2:249:LYS:O	2.16	0.45
1:2:268:LYS:HZ2	1:2:268:LYS:HB3	1.81	0.45
1:2:89:LYS:O	1:2:93:GLU:HB2	2.16	0.45
1:2:182:TYR:CD2	1:2:191:GLU:HG2	2.51	0.45
1:4:165:LEU:O	1:4:209:PHE:HA	2.17	0.45
1:3:245:VAL:HG21	3:3:716:HOH:O	2.17	0.45
1:1:230:ASN:H	1:1:230:ASN:HD22	1.65	0.45
1:4:110:LEU:HD12	1:4:296:PRO:O	2.17	0.45
1:2:131:TRP:HB3	1:2:256:MET:HG3	1.97	0.45
1:1:282:ASP:O	1:1:286:GLN:HB2	2.17	0.45
1:1:310:ASN:ND2	1:1:310:ASN:O	2.50	0.45
1:4:301:ARG:NH2	1:4:315:TYR:HB3	2.32	0.45
1:1:81:VAL:HG22	1:1:259:LEU:HD23	1.98	0.45
1:3:93:GLU:HG2	1:3:95:MET:SD	2.57	0.45
1:4:150:SER:HB2	1:4:250:GLU:OE2	2.17	0.45
1:4:68:LYS:CE	1:4:72:TYR:HB2	2.47	0.45
1:3:177:LEU:C	1:3:183:SER:HB3	2.37	0.44
1:2:174:GLN:O	1:2:178:ARG:HG3	2.17	0.44
1:4:186:THR:HG22	1:4:188:ASP:N	2.32	0.44
1:4:111:ASP:OD2	1:4:113:ASP:HB2	2.17	0.44
1:1:38:VAL:HG13	1:1:56:TYR:OH	2.16	0.44
1:4:165:LEU:HA	1:4:227:MET:CG	2.47	0.44
1:4:176:ALA:HB2	1:4:199:LEU:CD2	2.48	0.44
1:2:304:LEU:HD21	1:2:315:TYR:CZ	2.52	0.44
1:3:151:TRP:CA	1:3:154:LEU:HD13	2.47	0.44
1:1:48:LYS:HZ2	1:1:48:LYS:HA	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:161:GLY:N	1:1:205:ASN:HA	2.31	0.44
1:2:180:LEU:HG	1:2:198:GLU:OE2	2.17	0.44
1:4:280:ARG:NH1	1:4:282:ASP:OD2	2.51	0.44
1:3:293:TYR:HA	1:3:294:PRO:HD3	1.80	0.44
1:2:305:SER:HA	1:2:306:PRO:HD3	1.79	0.44
1:2:160:LYS:CA	1:2:205:ASN:ND2	2.69	0.44
1:1:79:LEU:HD21	1:1:259:LEU:HD22	1.98	0.44
1:3:74:ASP:N	1:3:74:ASP:OD1	2.50	0.44
1:1:129:TYR:HB2	1:1:259:LEU:HG	1.99	0.44
1:4:149:THR:O	1:4:249:LYS:N	2.51	0.44
1:4:171:GLU:OE2	2:4:400:SPD:N10	2.50	0.44
1:1:228:ILE:HG12	1:1:229:TRP:N	2.31	0.44
1:2:26:ASN:C	1:2:26:ASN:OD1	2.56	0.44
1:1:68:LYS:HE3	1:1:68:LYS:HA	2.00	0.44
1:2:34:TRP:HA	1:2:59:TYR:O	2.18	0.44
1:2:80:VAL:CG1	1:2:81:VAL:N	2.80	0.44
1:3:101:LYS:CA	1:3:101:LYS:HZ2	2.31	0.44
1:1:181:GLY:O	1:1:183:SER:OG	2.31	0.44
1:1:180:LEU:CD1	1:1:182:TYR:CE2	2.94	0.44
1:4:180:LEU:HD11	1:4:198:GLU:CD	2.37	0.44
1:2:348:ARG:HD2	1:2:348:ARG:C	2.37	0.44
1:4:268:LYS:O	1:4:272:LEU:HD23	2.17	0.44
1:2:166:THR:HG21	1:2:171:GLU:OE1	2.18	0.44
1:3:177:LEU:HD12	1:3:182:TYR:O	2.17	0.44
1:2:177:LEU:HD12	1:2:195:ALA:HB2	1.99	0.44
1:3:166:THR:H	1:3:227:MET:HG3	1.82	0.44
1:3:306:PRO:O	1:3:310:ASN:HB2	2.17	0.44
1:2:255:TRP:CH2	2:2:400:SPD:H52	2.52	0.44
1:4:166:THR:HB	1:4:227:MET:HE2	2.00	0.44
1:4:155:TRP:CZ2	1:4:202:LEU:HD23	2.53	0.44
1:4:89:LYS:HA	1:4:92:LYS:HE2	2.00	0.44
1:2:117:LYS:HB3	1:2:119:PHE:CE1	2.53	0.44
1:4:74:ASP:HB3	3:4:573:HOH:O	2.16	0.44
1:4:202:LEU:O	1:4:205:ASN:HB2	2.18	0.44
1:4:224:ASN:HA	1:4:224:ASN:HD22	1.68	0.44
1:2:245:VAL:HB	1:2:313:THR:HG21	2.00	0.43
1:2:234:PHE:CD1	1:2:314:LEU:HD11	2.53	0.43
1:1:165:LEU:HA	1:1:227:MET:HG3	2.00	0.43
1:2:168:ASP:O	1:2:172:VAL:HG23	2.18	0.43
1:1:133:ALA:HB2	1:1:254:PHE:CD1	2.53	0.43
1:3:141:ASP:HB2	1:3:242:PRO:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:131:TRP:HA	1:1:256:MET:HA	1.99	0.43
1:2:178:ARG:NH1	1:2:325:GLU:HB2	2.33	0.43
1:2:27:ASN:CG	1:2:28:THR:N	2.72	0.43
1:1:253:ILE:H	1:1:253:ILE:HG13	1.54	0.43
1:1:228:ILE:HD12	1:1:243:ILE:CD1	2.48	0.43
1:1:153:ASP:O	1:1:159:TYR:CE2	2.71	0.43
1:3:79:LEU:HD12	1:3:260:ALA:O	2.17	0.43
1:2:293:TYR:HA	1:2:294:PRO:HD3	1.89	0.43
1:1:301:ARG:HG2	1:1:301:ARG:NH1	2.32	0.43
1:2:269:GLU:HG3	3:2:632:HOH:O	2.19	0.43
1:2:83:SER:OG	2:2:400:SPD:H82	2.17	0.43
1:3:90:MET:O	1:3:95:MET:N	2.46	0.43
1:3:236:ALA:O	1:3:239:ALA:HB3	2.19	0.43
1:1:182:TYR:HD2	1:1:191:GLU:HB3	1.83	0.43
1:3:164:LEU:HD13	1:3:165:LEU:N	2.33	0.43
1:4:177:LEU:HD13	1:4:195:ALA:CB	2.47	0.43
1:2:38:VAL:CG2	1:2:38:VAL:O	2.67	0.43
1:2:139:ASN:ND2	3:2:639:HOH:O	2.48	0.43
1:2:72:TYR:CE1	1:2:74:ASP:OD1	2.71	0.43
1:4:186:THR:HG22	1:4:188:ASP:H	1.82	0.43
1:1:156:LYS:HB2	1:1:159:TYR:CE2	2.54	0.43
1:1:145:PRO:O	1:1:148:VAL:HG22	2.19	0.43
1:1:62:ASN:HD22	1:1:62:ASN:H	1.65	0.43
1:4:133:ALA:HB2	1:4:254:PHE:HD1	1.82	0.43
1:1:185:ASN:HD22	1:1:328:ASN:CA	2.32	0.43
1:4:228:ILE:CD1	1:4:243:ILE:HD11	2.46	0.43
1:2:301:ARG:O	1:2:304:LEU:HB2	2.19	0.43
1:2:72:TYR:CD1	1:2:73:LYS:N	2.86	0.43
1:1:182:TYR:CD2	1:1:191:GLU:HB3	2.53	0.43
1:4:165:LEU:HD13	1:4:206:VAL:HG22	2.00	0.43
1:2:259:LEU:HD13	1:2:275:ILE:HG23	2.01	0.43
1:4:332:ALA:O	1:4:334:SER:N	2.52	0.43
1:3:133:ALA:HA	1:3:253:ILE:O	2.19	0.42
1:3:26:ASN:OD1	1:3:27:ASN:N	2.52	0.42
1:4:252:GLY:N	3:4:541:HOH:O	2.51	0.42
1:3:340:TYR:HD1	1:3:343:LYS:HD2	1.85	0.42
1:4:134:THR:HB	1:4:253:ILE:HB	2.01	0.42
1:2:331:GLY:C	1:2:333:ALA:H	2.22	0.42
1:2:177:LEU:CD1	1:2:195:ALA:HB2	2.49	0.42
1:3:247:TRP:HE1	1:3:312:LYS:HG3	1.84	0.42
1:2:74:ASP:HA	3:2:616:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:298:LEU:O	1:3:302:LYS:HG3	2.19	0.42
1:2:133:ALA:HB2	1:2:254:PHE:CD1	2.54	0.42
1:1:199:LEU:HB3	1:1:344:LEU:HD11	2.01	0.42
1:2:164:LEU:HB2	1:2:223:VAL:HG11	2.01	0.42
1:4:156:LYS:HA	1:4:157:PRO:HD3	1.79	0.42
1:4:161:GLY:O	1:4:207:ALA:HB2	2.19	0.42
1:1:300:ALA:HA	1:1:303:LEU:HD22	2.01	0.42
1:3:178:ARG:CZ	1:3:250:GLU:O	2.67	0.42
1:4:317:ASP:N	1:4:317:ASP:OD1	2.44	0.42
1:2:185:ASN:HD22	1:2:328:ASN:HB2	1.81	0.42
1:4:177:LEU:HD12	1:4:177:LEU:HA	1.86	0.42
1:2:77:TYR:O	1:2:262:PRO:CG	2.67	0.42
1:3:230:ASN:ND2	1:3:230:ASN:N	2.66	0.42
1:3:224:ASN:HB2	3:3:576:HOH:O	2.19	0.42
1:4:27:ASN:O	1:4:52:ILE:HG23	2.19	0.42
1:4:75:GLY:O	1:4:76:ALA:HB2	2.20	0.42
1:3:304:LEU:HD21	1:3:315:TYR:OH	2.19	0.42
1:1:262:PRO:O	1:1:264:ASN:N	2.53	0.42
1:2:122:ASN:ND2	1:2:122:ASN:H	2.17	0.42
1:2:52:ILE:HD12	1:2:273:LYS:HD2	2.01	0.42
1:2:279:LEU:HA	3:2:521:HOH:O	2.19	0.42
1:4:305:SER:HA	1:4:306:PRO:HD3	1.78	0.42
1:2:73:LYS:C	1:2:75:GLY:H	2.24	0.42
1:3:117:LYS:HA	1:3:118:PRO:HD3	1.66	0.42
1:3:219:MET:O	1:4:57:SER:HA	2.20	0.42
1:2:159:TYR:CB	1:2:163:LEU:HD11	2.44	0.41
1:4:91:ARG:HD2	1:4:125:TYR:CE1	2.55	0.41
1:3:266:LYS:HA	1:3:266:LYS:HE3	2.02	0.41
1:3:101:LYS:HA	1:3:104:LEU:CD2	2.48	0.41
1:3:214:PRO:HG2	1:3:229:TRP:CE3	2.55	0.41
1:2:36:GLU:OE2	2:2:400:SPD:N1	2.53	0.41
1:4:59:TYR:CZ	1:4:65:MET:HG3	2.56	0.41
1:1:190:LYS:HB3	1:1:190:LYS:HE2	1.89	0.41
1:1:72:TYR:HD1	1:1:73:LYS:N	2.18	0.41
1:2:276:ASN:HD22	1:2:276:ASN:HA	1.68	0.41
1:4:29:LEU:O	1:4:54:VAL:HA	2.20	0.41
1:3:136:ILE:HG21	1:3:148:VAL:HG11	2.02	0.41
1:4:38:VAL:O	1:4:38:VAL:CG2	2.68	0.41
1:2:230:ASN:N	1:2:230:ASN:HD22	2.17	0.41
1:2:165:LEU:HD11	1:2:202:LEU:HD21	2.02	0.41
1:3:135:ALA:HB1	1:3:246:VAL:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:151:TRP:HB3	1:1:175:MET:HG3	2.02	0.41
1:3:323:ASN:HD22	1:3:323:ASN:C	2.22	0.41
1:1:185:ASN:O	1:1:330:VAL:HG12	2.20	0.41
1:4:117:LYS:HD3	1:4:117:LYS:N	2.35	0.41
1:1:236:ALA:O	1:1:239:ALA:HB3	2.20	0.41
1:4:26:ASN:HB3	3:4:714:HOH:O	2.20	0.41
1:4:176:ALA:HB2	1:4:199:LEU:HD21	2.03	0.41
1:2:136:ILE:HD11	1:2:248:PRO:HB3	2.02	0.41
1:1:228:ILE:HG12	1:1:229:TRP:H	1.86	0.41
1:4:32:TYR:CB	1:4:76:ALA:CB	2.97	0.41
1:3:254:PHE:HE2	1:3:324:GLY:HA3	1.86	0.41
1:3:106:ASN:O	1:3:109:ASN:ND2	2.54	0.41
1:1:178:ARG:N	1:1:183:SER:HB3	2.36	0.41
1:1:32:TYR:CG	1:1:76:ALA:CB	3.04	0.41
1:2:117:LYS:CD	1:2:117:LYS:N	2.79	0.41
1:1:200:LYS:C	1:1:202:LEU:H	2.24	0.41
1:2:213:ASN:HD21	1:2:216:ASN:HD22	1.69	0.41
1:2:203:MET:N	1:2:204:PRO:HD2	2.35	0.41
1:3:111:ASP:OD1	1:3:114:MET:HG3	2.20	0.41
1:4:289:GLU:HG2	1:4:308:VAL:HG21	2.03	0.41
1:4:127:ILE:O	1:4:128:PRO:C	2.60	0.41
1:1:318:ALA:C	1:1:321:ILE:HG12	2.41	0.41
1:1:117:LYS:HA	1:1:118:PRO:HD3	1.76	0.41
1:4:185:ASN:ND2	1:4:328:ASN:HB2	2.36	0.41
1:1:68:LYS:HE3	1:1:72:TYR:HB2	2.03	0.40
1:4:106:ASN:O	1:4:109:ASN:HB2	2.21	0.40
1:3:267:ASN:C	1:3:267:ASN:HD22	2.24	0.40
1:1:295:THR:HA	1:1:296:PRO:HD3	1.86	0.40
1:1:180:LEU:CD1	1:1:180:LEU:C	2.90	0.40
1:3:237:ARG:NH1	3:3:716:HOH:O	2.48	0.40
1:3:150:SER:HB2	1:3:250:GLU:OE1	2.21	0.40
1:3:106:ASN:HB2	1:3:276:ASN:ND2	2.37	0.40
1:3:203:MET:HA	1:3:206:VAL:HG23	2.04	0.40
1:4:196:TYR:OH	1:4:343:LYS:HB2	2.22	0.40
1:4:166:THR:HB	1:4:227:MET:CE	2.51	0.40
1:2:117:LYS:HA	1:2:118:PRO:HD3	1.77	0.40
1:3:168:ASP:O	1:3:172:VAL:HG23	2.22	0.40
1:3:122:ASN:ND2	1:3:122:ASN:N	2.69	0.40
1:1:318:ALA:CA	1:1:321:ILE:HG12	2.51	0.40
1:4:36:GLU:HG2	1:4:36:GLU:H	1.70	0.40
1:1:162:SER:N	1:1:205:ASN:O	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:42:LEU:HD11	1:4:283:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	321/323 (99%)	276 (86%)	42 (13%)	3 (1%)	21	37
1	2	321/323 (99%)	283 (88%)	35 (11%)	3 (1%)	21	37
1	3	321/323 (99%)	287 (89%)	29 (9%)	5 (2%)	12	21
1	4	321/323 (99%)	277 (86%)	39 (12%)	5 (2%)	12	21
All	All	1284/1292 (99%)	1123 (88%)	145 (11%)	16 (1%)	16	29

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	184	GLY
1	3	35	THR
1	3	123	ASN
1	4	35	THR
1	3	36	GLU
1	3	76	ALA
1	3	317	ASP
1	4	76	ALA
1	1	263	ALA
1	2	242	PRO
1	4	333	ALA
1	1	149	THR
1	4	36	GLU
1	4	108	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	76	ALA
1	2	74	ASP

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	1	272/273 (100%)	221 (81%)	51 (19%)	2	3
1	2	273/273 (100%)	219 (80%)	54 (20%)	1	3
1	3	273/273 (100%)	224 (82%)	49 (18%)	2	3
1	4	273/273 (100%)	223 (82%)	50 (18%)	2	3
All	All	1091/1092 (100%)	887 (81%)	204 (19%)	2	3

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	28	THR
1	1	32	TYR
1	1	33	ASN
1	1	36	GLU
1	1	38	VAL
1	1	48	LYS
1	1	54	VAL
1	1	57	SER
1	1	68	LYS
1	1	72	TYR
1	1	74	ASP
1	1	84	THR
1	1	86	TYR
1	1	89	LYS
1	1	93	GLU
1	1	101	LYS
1	1	110	LEU
1	1	111	ASP
1	1	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	117	LYS
1	1	121	PRO
1	1	123	ASN
1	1	138	VAL
1	1	146	LYS
1	1	158	GLU
1	1	166	THR
1	1	167	ASP
1	1	168	ASP
1	1	174	GLN
1	1	177	LEU
1	1	182	TYR
1	1	185	ASN
1	1	198	GLU
1	1	199	LEU
1	1	216	ASN
1	1	227	MET
1	1	228	ILE
1	1	230	ASN
1	1	238	GLN
1	1	262	PRO
1	1	267	ASN
1	1	278	LEU
1	1	291	ILE
1	1	303	LEU
1	1	304	LEU
1	1	310	ASN
1	1	319	GLU
1	1	322	LYS
1	1	342	GLN
1	1	343	LYS
1	1	348	ARG
1	2	28	THR
1	2	32	TYR
1	2	36	GLU
1	2	38	VAL
1	2	43	LEU
1	2	44	GLU
1	2	57	SER
1	2	65	MET
1	2	68	LYS
1	2	69	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	72	TYR
1	2	73	LYS
1	2	83	SER
1	2	84	THR
1	2	86	TYR
1	2	93	GLU
1	2	98	LYS
1	2	101	LYS
1	2	104	LEU
1	2	111	ASP
1	2	117	LYS
1	2	122	ASN
1	2	123	ASN
1	2	138	VAL
1	2	146	LYS
1	2	154	LEU
1	2	158	GLU
1	2	165	LEU
1	2	168	ASP
1	2	174	GLN
1	2	180	LEU
1	2	211	SER
1	2	216	ASN
1	2	225	LEU
1	2	227	MET
1	2	230	ASN
1	2	238	GLN
1	2	264	ASN
1	2	267	ASN
1	2	276	ASN
1	2	278	LEU
1	2	285	LYS
1	2	290	THR
1	2	295	THR
1	2	303	LEU
1	2	304	LEU
1	2	310	ASN
1	2	312	LYS
1	2	319	GLU
1	2	323	ASN
1	2	335	SER
1	2	338	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	340	TYR
1	2	342	GLN
1	3	28	THR
1	3	32	TYR
1	3	36	GLU
1	3	48	LYS
1	3	54	VAL
1	3	68	LYS
1	3	72	TYR
1	3	74	ASP
1	3	84	THR
1	3	86	TYR
1	3	89	LYS
1	3	90	MET
1	3	98	LYS
1	3	101	LYS
1	3	104	LEU
1	3	114	MET
1	3	116	ASN
1	3	122	ASN
1	3	138	VAL
1	3	141	ASP
1	3	146	LYS
1	3	147	SER
1	3	157	PRO
1	3	158	GLU
1	3	163	LEU
1	3	165	LEU
1	3	177	LEU
1	3	185	ASN
1	3	186	THR
1	3	199	LEU
1	3	211	SER
1	3	217	PRO
1	3	230	ASN
1	3	238	GLN
1	3	264	ASN
1	3	266	LYS
1	3	267	ASN
1	3	269	GLU
1	3	272	LEU
1	3	278	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	285	LYS
1	3	287	VAL
1	3	290	THR
1	3	295	THR
1	3	304	LEU
1	3	312	LYS
1	3	323	ASN
1	3	342	GLN
1	3	345	LYS
1	4	32	TYR
1	4	48	LYS
1	4	54	VAL
1	4	68	LYS
1	4	72	TYR
1	4	84	THR
1	4	86	TYR
1	4	89	LYS
1	4	98	LYS
1	4	101	LYS
1	4	104	LEU
1	4	108	SER
1	4	110	LEU
1	4	113	ASP
1	4	123	ASN
1	4	124	ASP
1	4	154	LEU
1	4	158	GLU
1	4	160	LYS
1	4	165	LEU
1	4	166	THR
1	4	168	ASP
1	4	174	GLN
1	4	177	LEU
1	4	182	TYR
1	4	183	SER
1	4	187	THR
1	4	190	LYS
1	4	196	TYR
1	4	202	LEU
1	4	205	ASN
1	4	211	SER
1	4	216	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4	230	ASN
1	4	238	GLN
1	4	267	ASN
1	4	276	ASN
1	4	278	LEU
1	4	285	LYS
1	4	295	THR
1	4	302	LYS
1	4	310	ASN
1	4	311	ASP
1	4	317	ASP
1	4	319	GLU
1	4	323	ASN
1	4	329	ASP
1	4	338	GLU
1	4	340	TYR
1	4	348	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	26	ASN
1	1	33	ASN
1	1	109	ASN
1	1	174	GLN
1	1	185	ASN
1	1	205	ASN
1	1	230	ASN
1	1	267	ASN
1	1	276	ASN
1	1	323	ASN
1	1	342	GLN
1	2	27	ASN
1	2	33	ASN
1	2	116	ASN
1	2	122	ASN
1	2	174	GLN
1	2	197	ASN
1	2	205	ASN
1	2	216	ASN
1	2	230	ASN
1	2	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	276	ASN
1	3	27	ASN
1	3	33	ASN
1	3	45	GLN
1	3	116	ASN
1	3	122	ASN
1	3	205	ASN
1	3	213	ASN
1	3	216	ASN
1	3	230	ASN
1	3	267	ASN
1	3	276	ASN
1	3	323	ASN
1	3	328	ASN
1	3	342	GLN
1	4	33	ASN
1	4	45	GLN
1	4	106	ASN
1	4	174	GLN
1	4	197	ASN
1	4	213	ASN
1	4	224	ASN
1	4	230	ASN
1	4	267	ASN
1	4	276	ASN
1	4	323	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

4 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
2	SPD	1	400	-	9,9,9	0.63	0	8,8,8	1.50	1 (12%)
2	SPD	2	400	-	9,9,9	0.58	0	8,8,8	2.89	3 (37%)
2	SPD	3	400	-	9,9,9	0.63	0	8,8,8	1.15	1 (12%)
2	SPD	4	400	-	9,9,9	0.98	1 (11%)	8,8,8	1.78	2 (25%)

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
2	SPD	1	400	-	-	0/7/7/7	0/0/0/0
2	SPD	2	400	-	-	0/7/7/7	0/0/0/0
2	SPD	3	400	-	-	0/7/7/7	0/0/0/0
2	SPD	4	400	-	-	0/7/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	400	SPD	C7-N6	-2.56	1.38	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	400	SPD	C4-C5-N6	-3.92	102.17	111.96
2	1	400	SPD	C7-N6-C5	-3.76	100.05	113.35
2	2	400	SPD	C7-N6-C5	-3.60	100.61	113.35
2	2	400	SPD	C4-C5-N6	-3.06	104.32	111.96
2	3	400	SPD	C4-C5-N6	-2.75	105.09	111.96
2	4	400	SPD	C8-C7-N6	2.76	118.85	111.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	400	SPD	C8-C7-N6	6.39	127.93	111.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	400	SPD	8	0
2	2	400	SPD	10	0
2	3	400	SPD	5	0
2	4	400	SPD	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1	323/323 (100%)	-1.34	0 100 100	7, 20, 33, 43	0
1	2	323/323 (100%)	-1.37	0 100 100	6, 19, 30, 41	0
1	3	323/323 (100%)	-1.38	0 100 100	6, 17, 27, 43	0
1	4	323/323 (100%)	-1.36	0 100 100	5, 18, 30, 46	0
All	All	1292/1292 (100%)	-1.37	0 100 100	5, 18, 31, 46	0

There are no RSRZ outliers to report.

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
2	SPD	2	400	10/10	0.95	0.10	3.67	18,26,34,37	0
2	SPD	4	400	10/10	0.93	0.09	3.10	14,21,22,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SPD	1	400	10/10	0.95	0.08	1.58	20,23,24,25	0
2	SPD	3	400	10/10	0.96	0.06	0.12	14,18,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.