



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 02:17 am BST

PDB ID : 2FO1
Title : Crystal Structure of the CSL-Notch-Mastermind ternary complex bound to DNA
Authors : Wilson, J.J.; Kovall, R.A.
Deposited on : 2006-01-12
Resolution : 3.12 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 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 : 2.11
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) : 2.11

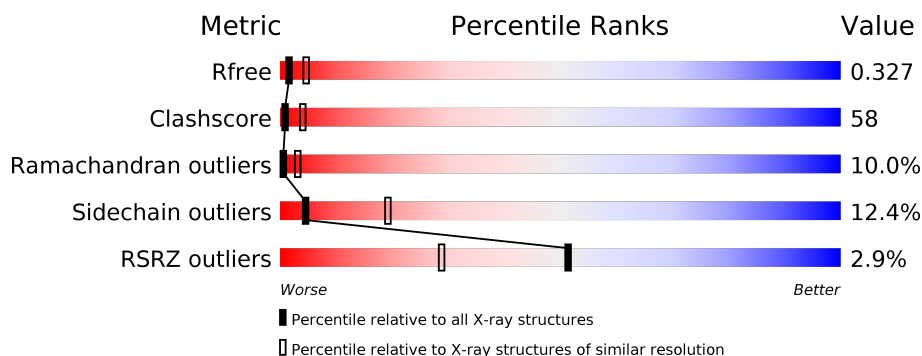
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	15	
2	C	15	
3	A	477	
4	D	85	
5	E	373	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6939 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 DNA chain called 5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			298	145	50	89	14			

- Molecule 3 is a protein called Lin-12 and glp-1 phenotype protein 1, isoform b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	439	Total	C	N	O	S	0	0	0
			3497	2218	608	654	17			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLY	-	CLONING ARTIFACT	GB 22532887
A	188	PRO	-	CLONING ARTIFACT	GB 22532887
A	189	LEU	-	CLONING ARTIFACT	GB 22532887
A	190	GLY	-	CLONING ARTIFACT	GB 22532887
A	191	SER	-	CLONING ARTIFACT	GB 22532887

- Molecule 4 is a protein called Protein lag-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	63	Total	C	N	O	S	0	0	0
			524	316	102	105	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	48	SER	-	CLONING ARTIFACT	UNP Q09260

- Molecule 5 is a protein called Lin-12 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	297	Total	C	N	O	S	Se	0	0	0
			2309	1420	427	445	3	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	929	GLY	-	CLONING ARTIFACT	UNP P14585
E	930	SER	-	CLONING ARTIFACT	UNP P14585
E	939	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	946	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	949	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1090	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1099	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1114	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1142	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1143	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1146	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1164	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1168	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1220	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1246	MSE	MET	MODIFIED RESIDUE	UNP P14585
E	1258	MSE	MET	MODIFIED RESIDUE	UNP P14585

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 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: 5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3'

Chain B: 



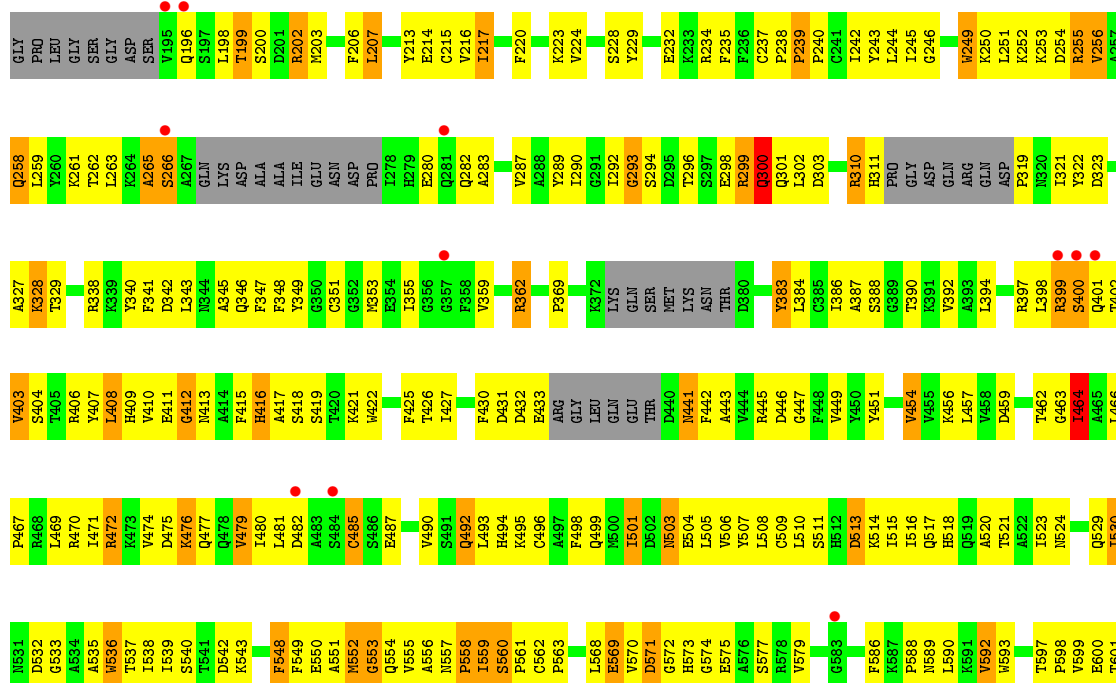
- Molecule 2: 5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3'

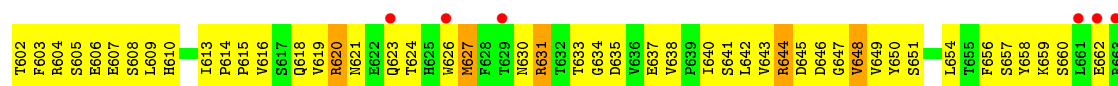
Chain C: 



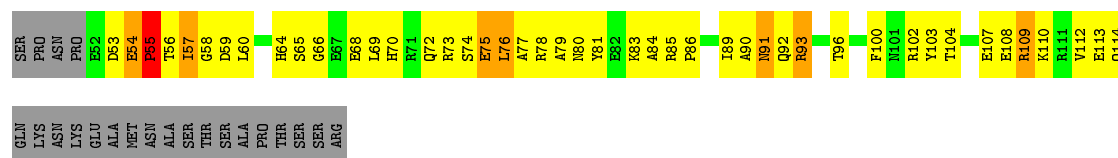
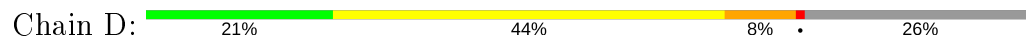
- Molecule 3: Lin-12 and glp-1 phenotype protein 1, isoform b

Chain A: 

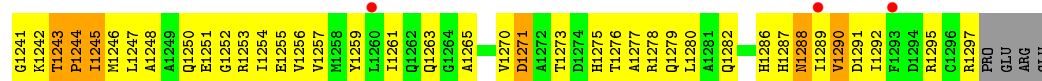
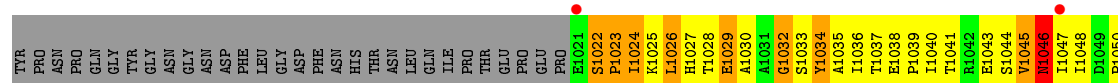
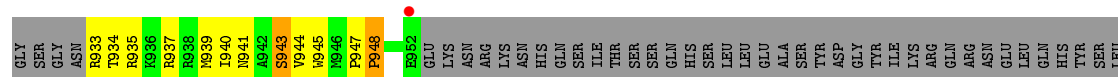
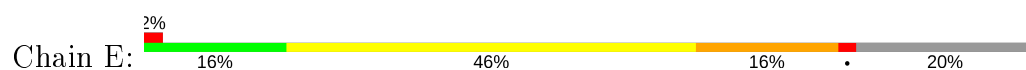




• Molecule 4: Protein lag-3



• Molecule 5: Lin-12 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.09 Å 96.78 Å 243.54 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.51 – 3.12 43.51 – 3.12	Depositor EDS
% Data completeness (in resolution range)	88.6 (43.51-3.12) 93.0 (43.51-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.12 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.273 , 0.340 0.276 , 0.327	Depositor DCC
R_{free} test set	4706 reflections (9.04%)	wwPDB-VP
Wilson B-factor (Å ²)	94.2	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6939	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.66	0/350	0.80	0/540
2	C	0.64	0/332	0.81	0/509
3	A	0.45	0/3573	0.70	0/4822
4	D	0.37	0/532	0.69	1/714 (0.1%)
5	E	0.42	0/2327	0.76	0/3113
All	All	0.46	0/7114	0.73	1/9698 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
2	C	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	54	GLU	C-N-CD	-5.81	107.83	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	12	DA	Sidechain
1	B	2	DT	Sidechain
2	C	2	DA	Sidechain
2	C	5	DT	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	B	311	0	171	20	0
2	C	298	0	172	17	0
3	A	3497	0	3441	343	0
4	D	524	0	491	51	0
5	E	2309	0	2301	392	0
All	All	6939	0	6576	785	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 58.

All (785) 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)
5:E:1022:SER:H	5:E:1023:PRO:HD2	1.17	1.08
5:E:1167:LEU:HD12	5:E:1167:LEU:H	1.14	1.07
3:A:283:ALA:HB1	3:A:351:CYS:HB3	1.33	1.07
5:E:935:ARG:NH1	5:E:1158:GLU:HG2	1.69	1.06
2:C:8:DC:H2''	2:C:9:DC:H5'	1.33	1.04
3:A:328:LYS:H	3:A:328:LYS:HD3	1.20	1.04
5:E:1057:LEU:HD12	5:E:1057:LEU:H	1.19	1.03
5:E:1037:THR:HG22	5:E:1038:GLU:H	1.24	1.01
5:E:1063:ASN:ND2	5:E:1106:ARG:HD3	1.74	1.01
5:E:1098:LEU:HD12	5:E:1098:LEU:O	1.58	1.01
3:A:293:GLY:HA3	3:A:338:ARG:HH22	1.25	0.99
3:A:479:VAL:HG12	3:A:481:LEU:HD23	1.39	0.99
5:E:1055:THR:H	5:E:1058:HIS:HD2	1.04	0.98
5:E:1055:THR:H	5:E:1058:HIS:CD2	1.83	0.97
5:E:1246:MSE:HE1	5:E:1271:ASP:HB3	1.43	0.97
3:A:631:ARG:H	3:A:631:ARG:HD2	1.27	0.96
5:E:1129:SER:H	5:E:1132:HIS:HD2	1.12	0.95
5:E:1034:TYR:HD1	5:E:1035:ALA:H	1.11	0.93
5:E:1120:PRO:HG2	5:E:1121:THR:H	1.32	0.93
5:E:1229:GLU:HG3	5:E:1230:LYS:N	1.81	0.93
5:E:1104:ALA:O	5:E:1105:ARG:HG2	1.70	0.92
5:E:1073:ILE:HD11	5:E:1106:ARG:CZ	1.98	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:DT:H2"	2:C:8:DC:H5"	1.53	0.91
4:D:54:GLU:HB3	4:D:55:PRO:HD2	1.51	0.91
5:E:1129:SER:H	5:E:1132:HIS:CD2	1.88	0.90
3:A:199:THR:HG23	3:A:202:ARG:HB2	1.51	0.90
3:A:472:ARG:HD3	3:A:499:GLN:OE1	1.72	0.90
3:A:328:LYS:N	3:A:328:LYS:HD3	1.88	0.89
5:E:1063:ASN:HD21	5:E:1106:ARG:HD3	1.37	0.89
5:E:1110:VAL:HG21	5:E:1142:MSE:HE1	1.55	0.88
5:E:1165:THR:O	5:E:1169:ILE:HG13	1.71	0.88
3:A:479:VAL:HG23	3:A:530:ILE:HD12	1.56	0.88
5:E:1119:ASP:OD1	5:E:1121:THR:HB	1.74	0.87
3:A:560:SER:HB3	3:A:561:PRO:HD3	1.56	0.87
3:A:293:GLY:HA3	3:A:338:ARG:NH2	1.90	0.87
5:E:1276:THR:HG22	5:E:1279:GLN:HE21	1.37	0.87
5:E:933:ARG:HH12	5:E:1090:MSE:SE	2.08	0.87
3:A:644:ARG:HB2	3:A:648:VAL:HG12	1.57	0.86
3:A:349:TYR:CE1	3:A:355:ILE:HD11	2.10	0.86
5:E:1156:ILE:HG21	5:E:1190:ALA:HB2	1.56	0.86
3:A:573:HIS:HB2	5:E:1104:ALA:HA	1.58	0.85
5:E:1167:LEU:N	5:E:1167:LEU:HD12	1.91	0.84
3:A:300:GLN:HG2	3:A:329:THR:OG1	1.78	0.84
3:A:388:SER:HB3	5:E:1202:SER:OG	1.76	0.84
3:A:479:VAL:HG12	3:A:479:VAL:O	1.77	0.84
5:E:1205:TYR:O	5:E:1206:LYS:CG	2.26	0.83
5:E:1045:VAL:HG23	5:E:1046:ASN:H	1.43	0.83
5:E:1245:ILE:H	5:E:1245:ILE:HD13	1.44	0.83
5:E:1114:MSE:HE2	5:E:1146:MSE:HG2	1.59	0.82
1:B:1:DT:H2'	1:B:2:DT:H71	1.61	0.82
3:A:292:ILE:C	3:A:294:SER:H	1.84	0.81
3:A:644:ARG:HB3	3:A:646:ASP:OD1	1.80	0.81
3:A:530:ILE:H	3:A:530:ILE:HD13	1.44	0.81
5:E:1114:MSE:HE1	5:E:1146:MSE:HA	1.62	0.81
5:E:1197:ALA:C	5:E:1199:ARG:H	1.83	0.80
3:A:355:ILE:O	3:A:559:ILE:HG12	1.82	0.80
3:A:427:ILE:HG23	3:A:427:ILE:O	1.82	0.79
3:A:283:ALA:CB	3:A:351:CYS:HB3	2.11	0.79
5:E:1074:VAL:O	5:E:1078:LYS:HG3	1.82	0.79
3:A:293:GLY:CA	3:A:338:ARG:HH22	1.96	0.79
5:E:1129:SER:N	5:E:1132:HIS:HD2	1.80	0.79
5:E:1099:MSE:HE1	5:E:1130:ALA:HA	1.63	0.79
5:E:1051:ARG:NH2	5:E:1051:ARG:HB2	1.97	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1205:TYR:O	5:E:1206:LYS:HG3	1.82	0.79
3:A:298:GLU:O	3:A:299:ARG:HB3	1.82	0.78
5:E:1141:GLY:HA2	5:E:1144:VAL:HG12	1.65	0.78
3:A:251:LEU:CD1	3:A:255:ARG:HD2	2.13	0.78
3:A:631:ARG:H	3:A:631:ARG:CD	1.96	0.77
5:E:1225:TYR:O	5:E:1229:GLU:HB3	1.84	0.77
2:C:7:DT:C2'	2:C:8:DC:H5''	2.15	0.77
5:E:1127:GLU:O	5:E:1160:ASP:HA	1.85	0.77
4:D:65:SER:O	4:D:69:LEU:HD13	1.85	0.77
3:A:199:THR:CG2	3:A:202:ARG:HB2	2.15	0.77
5:E:1056:VAL:O	5:E:1060:ILE:HG12	1.86	0.76
3:A:223:LYS:HD2	3:A:383:TYR:HE2	1.51	0.76
3:A:213:TYR:HB3	3:A:549:PHE:CE2	2.20	0.76
5:E:1037:THR:HG22	5:E:1038:GLU:N	2.00	0.76
5:E:1229:GLU:HG3	5:E:1230:LYS:H	1.47	0.76
5:E:934:THR:HG22	5:E:935:ARG:N	2.01	0.76
5:E:1237:GLN:HB3	5:E:1241:GLY:HA2	1.65	0.76
5:E:1128:ARG:HG2	5:E:1132:HIS:CB	2.15	0.76
5:E:1282:GLN:HG2	5:E:1290:VAL:HG22	1.67	0.75
3:A:432:ASP:H	3:A:443:ALA:HB3	1.50	0.75
5:E:1135:ALA:HA	5:E:1143:MSE:HE1	1.65	0.75
5:E:1217:VAL:HA	5:E:1253:ARG:CG	2.16	0.75
3:A:292:ILE:O	3:A:294:SER:N	2.17	0.75
3:A:579:VAL:HG23	3:A:613:ILE:HD11	1.67	0.75
5:E:1243:THR:HB	5:E:1245:ILE:HG12	1.68	0.75
5:E:934:THR:HG22	5:E:935:ARG:H	1.52	0.75
3:A:447:GLY:H	5:E:1202:SER:HB2	1.51	0.74
3:A:493:LEU:HD21	3:A:539:ILE:HD12	1.70	0.74
3:A:392:VAL:HG12	3:A:540:SER:HA	1.68	0.74
5:E:1051:ARG:HH21	5:E:1051:ARG:HB2	1.50	0.74
3:A:571:ASP:HB3	5:E:1133:GLN:HE22	1.52	0.73
4:D:86:PRO:HA	4:D:89:ILE:HG12	1.70	0.73
3:A:263:LEU:O	3:A:263:LEU:HD23	1.88	0.73
3:A:469:LEU:HB3	3:A:498:PHE:HB3	1.68	0.73
5:E:1141:GLY:HA2	5:E:1144:VAL:CG1	2.19	0.73
3:A:588:PRO:HG3	3:A:603:PHE:CG	2.24	0.73
2:C:8:DC:C2'	2:C:9:DC:H5'	2.15	0.73
5:E:1147:LEU:HG	5:E:1188:LYS:HG3	1.71	0.73
4:D:83:LYS:HD2	4:D:84:ALA:N	2.04	0.72
4:D:69:LEU:O	4:D:72:GLN:HB2	1.89	0.72
3:A:216:VAL:HB	3:A:245:ILE:HB	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1057:LEU:CD1	5:E:1057:LEU:H	1.99	0.72
3:A:397:ARG:C	3:A:398:LEU:HD22	2.11	0.71
5:E:1121:THR:HG22	5:E:1122:ILE:N	2.05	0.71
5:E:1288:ASN:O	5:E:1292:ILE:HG12	1.89	0.71
3:A:631:ARG:HD2	3:A:631:ARG:N	2.04	0.71
5:E:1055:THR:O	5:E:1058:HIS:HB2	1.89	0.71
4:D:89:ILE:O	4:D:93:ARG:HB2	1.88	0.71
5:E:1197:ALA:O	5:E:1199:ARG:N	2.23	0.71
5:E:1057:LEU:N	5:E:1057:LEU:HD12	2.00	0.71
3:A:387:ALA:HB3	3:A:390:THR:CG2	2.21	0.71
4:D:56:THR:HG23	5:E:1106:ARG:CZ	2.20	0.71
5:E:1218:SER:H	5:E:1253:ARG:HG3	1.55	0.71
3:A:569:GLU:HG2	5:E:1128:ARG:NH2	2.06	0.71
5:E:1062:SER:C	5:E:1064:SER:H	1.92	0.71
5:E:1024:ILE:HG22	5:E:1027:HIS:H	1.55	0.70
5:E:1072:LEU:HD12	5:E:1073:ILE:N	2.06	0.70
5:E:1114:MSE:HE3	5:E:1145:TYR:HE2	1.57	0.70
3:A:604:ARG:HH21	3:A:604:ARG:HG2	1.57	0.70
2:C:7:DT:H2''	2:C:8:DC:C5'	2.22	0.70
3:A:387:ALA:HB3	3:A:390:THR:HG23	1.74	0.70
4:D:54:GLU:CB	4:D:55:PRO:HD2	2.15	0.70
5:E:1098:LEU:O	5:E:1101:ALA:HB3	1.91	0.70
5:E:1147:LEU:HB3	5:E:1188:LYS:HE3	1.73	0.70
3:A:293:GLY:CA	3:A:338:ARG:HH12	2.05	0.69
3:A:298:GLU:O	3:A:299:ARG:CB	2.41	0.69
5:E:1100:LEU:HD12	5:E:1100:LEU:H	1.58	0.69
3:A:637:GLU:HA	3:A:656:PHE:O	1.92	0.69
5:E:1070:GLU:O	5:E:1073:ILE:HG12	1.91	0.69
5:E:1200:LYS:HA	5:E:1206:LYS:HD2	1.74	0.69
5:E:1201:ASP:CG	5:E:1202:SER:H	1.96	0.69
1:B:1:DT:C2'	1:B:2:DT:H71	2.22	0.69
5:E:1095:ASN:OD1	5:E:1099:MSE:HG2	1.93	0.69
3:A:223:LYS:HB2	3:A:540:SER:O	1.93	0.69
3:A:293:GLY:HA3	3:A:338:ARG:HH12	1.56	0.69
5:E:1138:ARG:HG3	5:E:1178:GLN:HE22	1.55	0.69
3:A:559:ILE:HA	3:A:644:ARG:HH22	1.56	0.69
3:A:568:LEU:HD23	3:A:568:LEU:C	2.13	0.68
5:E:1257:VAL:O	5:E:1261:ILE:HG12	1.92	0.68
3:A:442:PHE:CE2	3:A:456:LYS:HE2	2.28	0.68
4:D:70:HIS:CE1	5:E:1174:GLU:H	2.11	0.68
5:E:1045:VAL:HG12	5:E:1056:VAL:HG21	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1102:VAL:HG13	5:E:1142:MSE:HG2	1.74	0.68
3:A:425:PHE:HD2	3:A:459:ASP:HA	1.59	0.68
5:E:1205:TYR:O	5:E:1206:LYS:CB	2.41	0.68
3:A:415:PHE:HE1	3:A:464:ILE:HG23	1.58	0.68
3:A:548:PHE:HE1	3:A:559:ILE:HG13	1.59	0.68
1:B:13:DA:H1'	1:B:14:DG:H5''	1.76	0.68
5:E:1128:ARG:HG2	5:E:1132:HIS:HB2	1.76	0.68
3:A:560:SER:CB	3:A:561:PRO:HD3	2.24	0.68
3:A:557:ASN:HD22	3:A:557:ASN:N	1.91	0.67
5:E:1114:MSE:HE3	5:E:1145:TYR:CE2	2.29	0.67
5:E:1061:ALA:O	5:E:1063:ASN:N	2.27	0.67
3:A:310:ARG:HD2	3:A:311:HIS:H	1.58	0.67
5:E:1217:VAL:HA	5:E:1253:ARG:HG3	1.76	0.67
3:A:474:VAL:HG13	3:A:496:CYS:HA	1.77	0.67
5:E:1045:VAL:HG23	5:E:1046:ASN:N	2.10	0.67
5:E:1156:ILE:CG2	5:E:1190:ALA:HB2	2.24	0.67
5:E:1223:VAL:O	5:E:1227:VAL:HG22	1.94	0.67
5:E:1167:LEU:CD1	5:E:1167:LEU:H	1.96	0.67
5:E:1220:MSE:HA	5:E:1223:VAL:HG22	1.77	0.66
3:A:548:PHE:CE1	3:A:559:ILE:HG13	2.30	0.66
3:A:471:ILE:HG13	3:A:498:PHE:CE1	2.30	0.66
5:E:1077:ALA:O	5:E:1081:ILE:HG22	1.94	0.66
5:E:1098:LEU:HD12	5:E:1098:LEU:C	2.14	0.66
5:E:1120:PRO:CG	5:E:1121:THR:H	2.05	0.66
4:D:91:ASN:HD22	4:D:91:ASN:N	1.94	0.66
3:A:229:TYR:O	3:A:232:GLU:HG2	1.96	0.66
5:E:1297:ARG:HH11	5:E:1297:ARG:HB3	1.61	0.66
3:A:217:ILE:HD13	3:A:217:ILE:C	2.16	0.66
3:A:521:THR:OG1	3:A:529:GLN:HB2	1.95	0.66
4:D:107:GLU:OE1	4:D:110:LYS:HD2	1.94	0.65
5:E:1041:THR:H	5:E:1044:SER:CB	2.09	0.65
3:A:245:ILE:N	3:A:245:ILE:HD12	2.11	0.65
3:A:293:GLY:HA3	3:A:338:ARG:NH1	2.11	0.65
3:A:592:VAL:HG12	3:A:601:THR:OG1	1.96	0.65
5:E:1162:ASN:HB2	5:E:1164:MSE:HE2	1.78	0.65
3:A:431:ASP:HB3	3:A:443:ALA:HB1	1.78	0.65
4:D:76:LEU:HD11	5:E:1253:ARG:HH12	1.62	0.65
5:E:1132:HIS:O	5:E:1136:ALA:N	2.25	0.65
3:A:251:LEU:HD13	3:A:255:ARG:HD2	1.79	0.65
3:A:510:LEU:HD23	3:A:533:GLY:O	1.95	0.64
4:D:73:ARG:NH1	5:E:1218:SER:OG	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1055:THR:N	5:E:1058:HIS:HD2	1.86	0.64
3:A:447:GLY:N	5:E:1202:SER:HB2	2.12	0.64
5:E:1056:VAL:HG12	5:E:1060:ILE:HD11	1.80	0.64
5:E:1209:THR:O	5:E:1209:THR:HG23	1.97	0.64
3:A:459:ASP:OD1	3:A:462:THR:HG23	1.97	0.64
3:A:530:ILE:N	3:A:530:ILE:HD13	2.13	0.64
5:E:1104:ALA:C	5:E:1105:ARG:HG2	2.17	0.64
5:E:1234:LYS:HD3	5:E:1234:LYS:H	1.63	0.64
5:E:1282:GLN:HG2	5:E:1290:VAL:CG2	2.27	0.64
1:B:6:DG:H4'	3:A:235:PHE:HE2	1.61	0.64
3:A:237:CYS:HA	3:A:238:PRO:C	2.18	0.63
3:A:479:VAL:O	3:A:481:LEU:HD23	1.99	0.63
5:E:1157:GLU:O	5:E:1165:THR:HG22	1.97	0.63
3:A:509:CYS:SG	3:A:510:LEU:N	2.71	0.63
1:B:7:DT:H2''	1:B:8:DG:C8	2.34	0.63
5:E:1143:MSE:O	5:E:1147:LEU:HD22	1.98	0.63
5:E:1045:VAL:HG11	5:E:1080:CYS:CB	2.28	0.63
5:E:1197:ALA:C	5:E:1199:ARG:N	2.48	0.63
5:E:1202:SER:O	5:E:1203:GLU:C	2.37	0.63
3:A:551:ALA:HB3	3:A:647:GLY:O	1.99	0.62
3:A:621:ASN:H	3:A:624:THR:HG1	1.46	0.62
3:A:640:ILE:HD11	3:A:656:PHE:HB2	1.80	0.62
3:A:292:ILE:C	3:A:294:SER:N	2.51	0.62
5:E:1241:GLY:O	5:E:1271:ASP:HA	1.99	0.62
5:E:1217:VAL:HG23	5:E:1251:GLU:HB3	1.81	0.62
3:A:244:LEU:HB2	3:A:323:ASP:O	1.99	0.62
4:D:58:GLY:O	4:D:60:LEU:N	2.32	0.62
5:E:1120:PRO:HG2	5:E:1121:THR:N	2.10	0.62
2:C:14:DG:H2'	2:C:15:DT:C7	2.30	0.62
5:E:1139:ASP:OD2	5:E:1142:MSE:HB2	2.00	0.62
3:A:408:LEU:HD21	3:A:415:PHE:HD2	1.64	0.62
5:E:1243:THR:OG1	5:E:1246:MSE:HG3	1.99	0.62
5:E:1022:SER:N	5:E:1023:PRO:HD2	1.97	0.62
5:E:1245:ILE:HD13	5:E:1245:ILE:N	2.10	0.62
5:E:1040:ILE:HD12	5:E:1040:ILE:N	2.14	0.62
5:E:1091:ASP:OD2	5:E:1095:ASN:N	2.30	0.62
5:E:1270:VAL:HG12	5:E:1276:THR:HB	1.82	0.62
3:A:349:TYR:HE1	3:A:355:ILE:HD11	1.61	0.61
3:A:287:VAL:HB	3:A:348:PHE:CE1	2.35	0.61
3:A:560:SER:HB3	3:A:561:PRO:CD	2.30	0.61
5:E:1051:ARG:HH21	5:E:1051:ARG:CB	2.12	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1110:VAL:HG21	5:E:1142:MSE:CE	2.27	0.61
3:A:289:TYR:CE2	3:A:301:GLN:HB2	2.35	0.61
3:A:513:ASP:O	3:A:514:LYS:HG2	2.01	0.61
5:E:1078:LYS:HA	5:E:1081:ILE:CG2	2.29	0.61
3:A:388:SER:HB2	3:A:447:GLY:O	2.00	0.61
5:E:1220:MSE:HE3	5:E:1224:LYS:HG3	1.82	0.61
3:A:259:LEU:O	3:A:263:LEU:HB3	2.01	0.61
3:A:503:ASN:O	3:A:505:LEU:N	2.25	0.61
5:E:1030:ALA:HB1	5:E:1060:ILE:CD1	2.31	0.61
3:A:506:VAL:HA	3:A:518:HIS:O	2.01	0.60
3:A:213:TYR:HB3	3:A:549:PHE:CD2	2.35	0.60
4:D:70:HIS:HE1	5:E:1174:GLU:H	1.48	0.60
3:A:557:ASN:HB3	3:A:558:PRO:HD2	1.83	0.60
5:E:1133:GLN:HA	5:E:1136:ALA:HB3	1.83	0.60
5:E:1229:GLU:O	5:E:1230:LYS:HB2	2.00	0.60
3:A:293:GLY:HA3	3:A:338:ARG:CZ	2.30	0.60
3:A:548:PHE:HD2	3:A:548:PHE:O	1.85	0.60
3:A:586:PHE:HB2	3:A:606:GLU:O	2.01	0.60
1:B:3:DA:H1'	1:B:4:DC:H5'	1.83	0.60
4:D:55:PRO:O	5:E:1108:ARG:HB2	2.01	0.60
3:A:251:LEU:HD11	3:A:255:ARG:HD2	1.82	0.60
3:A:477:GLN:HG2	3:A:477:GLN:O	2.00	0.60
3:A:577:SER:HB3	3:A:613:ILE:HD13	1.83	0.60
5:E:1141:GLY:CA	5:E:1144:VAL:HG12	2.30	0.60
3:A:290:ILE:HD13	3:A:345:ALA:HB2	1.84	0.60
3:A:402:THR:O	3:A:404:SER:N	2.34	0.60
3:A:573:HIS:NE2	5:E:1064:SER:N	2.50	0.60
3:A:255:ARG:HH21	3:A:553:GLY:H	1.48	0.59
5:E:1133:GLN:NE2	5:E:1136:ALA:HB3	2.16	0.59
5:E:944:VAL:HG22	5:E:945:TRP:H	1.67	0.59
3:A:637:GLU:HA	3:A:657:SER:HA	1.83	0.59
1:B:1:DT:H2'	1:B:2:DT:C7	2.32	0.59
5:E:1096:THR:HG23	5:E:1099:MSE:H	1.67	0.59
3:A:552:MET:O	3:A:553:GLY:O	2.20	0.59
5:E:1037:THR:CG2	5:E:1038:GLU:H	2.04	0.59
1:B:6:DG:C8	1:B:7:DT:H72	2.38	0.59
5:E:1027:HIS:CE1	5:E:1048:ILE:HG22	2.37	0.59
3:A:506:VAL:HG11	3:A:517:GLN:HG2	1.84	0.59
4:D:104:THR:O	4:D:108:GLU:N	2.35	0.59
5:E:1102:VAL:HA	5:E:1142:MSE:HE3	1.85	0.59
3:A:633:THR:O	3:A:635:ASP:N	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1062:SER:C	5:E:1064:SER:N	2.56	0.58
5:E:1245:ILE:H	5:E:1245:ILE:CD1	2.06	0.58
3:A:644:ARG:O	3:A:646:ASP:N	2.31	0.58
5:E:1039:PRO:C	5:E:1040:ILE:HD12	2.24	0.58
5:E:1072:LEU:O	5:E:1076:GLU:N	2.27	0.58
5:E:1078:LYS:HA	5:E:1081:ILE:HG23	1.86	0.58
5:E:1133:GLN:HA	5:E:1133:GLN:NE2	2.18	0.58
5:E:1182:ALA:O	5:E:1186:VAL:HG12	2.03	0.58
3:A:494:HIS:O	3:A:537:THR:HA	2.04	0.58
5:E:1126:SER:HA	5:E:1161:ARG:HD2	1.85	0.58
5:E:944:VAL:HG22	5:E:945:TRP:N	2.18	0.58
4:D:109:ARG:O	4:D:113:GLU:HG2	2.03	0.58
3:A:520:ALA:HB1	3:A:530:ILE:HA	1.85	0.58
3:A:215:CYS:HB3	3:A:548:PHE:HE2	1.68	0.58
3:A:427:ILE:HD13	3:A:449:VAL:HG21	1.86	0.57
3:A:588:PRO:O	4:D:78:ARG:NH1	2.37	0.57
5:E:1086:ASP:O	5:E:1088:ASN:N	2.38	0.57
5:E:1045:VAL:O	5:E:1047:ILE:N	2.38	0.57
5:E:1064:SER:C	5:E:1066:ALA:H	2.07	0.57
3:A:252:LYS:NZ	3:A:554:GLN:HB2	2.19	0.57
5:E:1030:ALA:HB1	5:E:1060:ILE:HD13	1.87	0.57
5:E:1038:GLU:O	5:E:1040:ILE:CD1	2.53	0.57
3:A:479:VAL:HG12	3:A:481:LEU:CD2	2.25	0.57
5:E:1217:VAL:HA	5:E:1253:ARG:HG2	1.86	0.57
5:E:1246:MSE:O	5:E:1247:LEU:C	2.43	0.57
3:A:536:TRP:N	3:A:536:TRP:CD1	2.73	0.57
5:E:1022:SER:H	5:E:1023:PRO:CD	2.05	0.57
5:E:1200:LYS:O	5:E:1201:ASP:O	2.22	0.57
5:E:1287:HIS:O	5:E:1288:ASN:C	2.41	0.57
3:A:347:PHE:O	3:A:355:ILE:HB	2.05	0.57
3:A:559:ILE:HA	3:A:644:ARG:NH2	2.19	0.57
3:A:579:VAL:HG23	3:A:613:ILE:CD1	2.34	0.57
4:D:66:GLY:C	4:D:68:GLU:N	2.57	0.57
5:E:1270:VAL:HB	5:E:1275:HIS:O	2.05	0.56
3:A:252:LYS:HG3	3:A:349:TYR:OH	2.05	0.56
4:D:60:LEU:O	4:D:64:HIS:ND1	2.30	0.56
4:D:83:LYS:O	4:D:86:PRO:HD2	2.05	0.56
5:E:1045:VAL:HG11	5:E:1080:CYS:HB2	1.85	0.56
5:E:1220:MSE:SE	5:E:1223:VAL:HG21	2.56	0.56
5:E:1242:LYS:HZ2	5:E:1250:GLN:HE22	1.53	0.56
3:A:255:ARG:HH21	3:A:553:GLY:N	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:935:ARG:CB	5:E:1199:ARG:HH22	2.19	0.56
3:A:495:LYS:HA	3:A:536:TRP:O	2.05	0.56
5:E:1135:ALA:CA	5:E:1143:MSE:HE1	2.35	0.56
5:E:1167:LEU:O	5:E:1168:MSE:C	2.43	0.56
3:A:203:MET:HG3	3:A:207:LEU:HD12	1.87	0.56
3:A:479:VAL:CG1	3:A:479:VAL:O	2.51	0.56
5:E:945:TRP:CZ3	5:E:947:PRO:HB3	2.40	0.56
3:A:415:PHE:CE2	3:A:466:LEU:HG	2.40	0.56
5:E:1066:ALA:O	5:E:1067:GLU:HB3	2.06	0.56
5:E:1109:LEU:O	5:E:1113:LEU:HB2	2.04	0.56
3:A:441:ASN:HB2	5:E:939:MSE:HE1	1.87	0.56
5:E:1041:THR:O	5:E:1045:VAL:HG22	2.05	0.56
3:A:383:TYR:O	3:A:384:LEU:HD23	2.06	0.56
3:A:408:LEU:HB3	3:A:425:PHE:HE1	1.71	0.56
3:A:615:PRO:O	3:A:618:GLN:HG2	2.05	0.56
5:E:1062:SER:O	5:E:1064:SER:N	2.38	0.56
5:E:1186:VAL:HG11	5:E:1225:TYR:OH	2.05	0.55
5:E:934:THR:CG2	5:E:935:ARG:H	2.17	0.55
2:C:1:DA:H2"	2:C:2:DA:C8	2.41	0.55
3:A:557:ASN:ND2	3:A:557:ASN:N	2.54	0.55
2:C:13:DA:H2"	2:C:14:DG:H8	1.72	0.55
5:E:1087:VAL:HG22	5:E:1118:ALA:HB2	1.88	0.55
5:E:1109:LEU:HG	5:E:1113:LEU:HD23	1.88	0.55
5:E:1129:SER:N	5:E:1132:HIS:CD2	2.63	0.55
3:A:425:PHE:CD2	3:A:459:ASP:HA	2.40	0.55
5:E:1045:VAL:CG2	5:E:1046:ASN:H	2.09	0.55
3:A:548:PHE:O	3:A:548:PHE:CD2	2.60	0.55
4:D:100:PHE:O	4:D:103:TYR:HB3	2.05	0.55
3:A:228:SER:OG	3:A:234:ARG:HB2	2.06	0.55
5:E:1149:SER:O	5:E:1153:LYS:HD3	2.07	0.55
5:E:1197:ALA:HA	5:E:1200:LYS:HG3	1.87	0.55
5:E:1224:LYS:HA	5:E:1259:TYR:HE1	1.71	0.55
3:A:198:LEU:HD12	3:A:199:THR:H	1.72	0.55
3:A:362:ARG:HD2	3:A:362:ARG:N	2.21	0.55
4:D:76:LEU:HD13	4:D:77:ALA:N	2.22	0.55
5:E:1217:VAL:O	5:E:1218:SER:O	2.24	0.55
5:E:1242:LYS:NZ	5:E:1250:GLN:HE22	2.04	0.55
3:A:548:PHE:HD1	3:A:559:ILE:HG21	1.72	0.55
5:E:1081:ILE:C	5:E:1081:ILE:HD13	2.27	0.55
3:A:261:LYS:HG3	3:A:262:THR:N	2.22	0.55
3:A:220:PHE:HB3	3:A:422:TRP:CZ2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1114:MSE:CE	5:E:1146:MSE:HG2	2.32	0.55
5:E:1211:LEU:HD12	5:E:1211:LEU:O	2.07	0.55
3:A:588:PRO:HG3	3:A:603:PHE:CD2	2.42	0.54
4:D:75:GLU:OE1	4:D:75:GLU:HA	2.06	0.54
3:A:415:PHE:CE1	3:A:464:ILE:CG2	2.90	0.54
2:C:14:DG:OP1	2:C:14:DG:H4'	2.08	0.54
2:C:8:DC:H5'	2:C:8:DC:H6	1.71	0.54
5:E:1128:ARG:HG2	5:E:1132:HIS:HB3	1.89	0.54
5:E:1047:ILE:HD12	5:E:1047:ILE:N	2.22	0.54
3:A:259:LEU:O	3:A:263:LEU:CB	2.55	0.54
3:A:402:THR:HG23	3:A:403:VAL:H	1.72	0.54
3:A:586:PHE:HB2	3:A:606:GLU:C	2.28	0.54
3:A:599:VAL:HG12	3:A:600:GLU:N	2.22	0.54
1:B:6:DG:N2	3:A:400:SER:HB3	2.22	0.54
4:D:66:GLY:C	4:D:68:GLU:H	2.09	0.54
4:D:92:GLN:HE21	4:D:96:THR:HB	1.73	0.54
5:E:1140:PHE:CD1	5:E:1140:PHE:C	2.81	0.54
3:A:410:VAL:HG21	3:A:459:ASP:OD1	2.08	0.54
1:B:13:DA:C2'	1:B:14:DG:H5''	2.38	0.54
3:A:571:ASP:OD1	3:A:571:ASP:N	2.40	0.54
5:E:1201:ASP:CG	5:E:1202:SER:N	2.61	0.54
3:A:255:ARG:NH2	3:A:553:GLY:H	2.06	0.53
5:E:1133:GLN:HA	5:E:1136:ALA:CB	2.38	0.53
3:A:287:VAL:HG11	3:A:348:PHE:CZ	2.43	0.53
5:E:1245:ILE:O	5:E:1248:ALA:HB3	2.07	0.53
3:A:243:TYR:HB3	3:A:245:ILE:HD11	1.89	0.53
3:A:415:PHE:HE1	3:A:464:ILE:CG2	2.21	0.53
3:A:432:ASP:CG	3:A:433:GLU:H	2.11	0.53
5:E:935:ARG:CZ	5:E:1158:GLU:HG2	2.37	0.53
5:E:1238:ASP:OD1	5:E:1242:LYS:N	2.37	0.53
5:E:1096:THR:O	5:E:1100:LEU:HD12	2.08	0.53
5:E:1131:LEU:HD21	5:E:1185:LEU:HD21	1.90	0.53
5:E:1199:ARG:C	5:E:1201:ASP:N	2.60	0.53
3:A:572:GLY:N	5:E:1137:ASN:HD22	2.06	0.53
3:A:410:VAL:HG23	3:A:410:VAL:O	2.07	0.53
5:E:1057:LEU:HA	5:E:1060:ILE:HG12	1.90	0.53
5:E:1086:ASP:C	5:E:1088:ASN:H	2.11	0.53
5:E:1126:SER:O	5:E:1127:GLU:C	2.46	0.53
5:E:1200:LYS:HG2	5:E:1206:LYS:HD2	1.90	0.53
5:E:934:THR:CG2	5:E:935:ARG:N	2.69	0.53
3:A:613:ILE:H	3:A:613:ILE:HD12	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:ALA:HA	4:D:80:ASN:HD22	1.74	0.53
3:A:415:PHE:CE1	3:A:464:ILE:HG23	2.43	0.52
5:E:1027:HIS:HE1	5:E:1048:ILE:HG22	1.73	0.52
5:E:1048:ILE:N	5:E:1048:ILE:HD12	2.24	0.52
5:E:1159:LEU:H	5:E:1159:LEU:HD13	1.73	0.52
5:E:1203:GLU:HB3	5:E:1205:TYR:CD1	2.44	0.52
3:A:199:THR:HG23	3:A:202:ARG:H	1.74	0.52
3:A:442:PHE:CZ	3:A:456:LYS:HG2	2.45	0.52
2:C:14:DG:H2'	2:C:15:DT:H72	1.90	0.52
4:D:91:ASN:HD22	4:D:91:ASN:H	1.57	0.52
5:E:1167:LEU:O	5:E:1170:VAL:N	2.42	0.52
3:A:262:THR:O	3:A:262:THR:HG22	2.08	0.52
5:E:1196:GLY:O	5:E:1199:ARG:HB2	2.10	0.52
3:A:479:VAL:HG11	3:A:507:TYR:OH	2.10	0.52
5:E:1254:ILE:HG22	5:E:1289:ILE:HG12	1.92	0.52
3:A:369:PRO:HG3	3:A:493:LEU:HD12	1.92	0.52
3:A:432:ASP:O	3:A:433:GLU:CB	2.57	0.52
5:E:1046:ASN:HB3	5:E:1047:ILE:HD12	1.90	0.52
3:A:626:TRP:O	3:A:627:MET:HB2	2.10	0.52
5:E:1209:THR:O	5:E:1211:LEU:N	2.43	0.52
3:A:249:TRP:HA	3:A:249:TRP:CE3	2.45	0.51
5:E:1045:VAL:HG11	5:E:1080:CYS:HB3	1.91	0.51
3:A:542:ASP:CG	3:A:543:LYS:H	2.14	0.51
3:A:590:LEU:HA	3:A:643:VAL:O	2.10	0.51
5:E:945:TRP:CH2	5:E:947:PRO:HB3	2.45	0.51
5:E:1038:GLU:O	5:E:1040:ILE:HD12	2.10	0.51
5:E:1131:LEU:HD21	5:E:1185:LEU:CD2	2.40	0.51
3:A:509:CYS:O	3:A:515:ILE:HG23	2.11	0.51
5:E:1184:LEU:HD13	5:E:1184:LEU:C	2.31	0.51
5:E:1242:LYS:HG2	5:E:1246:MSE:HE2	1.93	0.51
5:E:1098:LEU:HD13	5:E:1110:VAL:HG13	1.92	0.51
5:E:1214:ALA:O	5:E:1215:ALA:C	2.49	0.51
4:D:56:THR:HG22	4:D:57:ILE:HD13	1.92	0.51
5:E:1159:LEU:HD23	5:E:1163:GLY:HA2	1.93	0.51
5:E:1220:MSE:O	5:E:1223:VAL:HG22	2.11	0.51
5:E:1235:ASP:HA	5:E:1243:THR:HG22	1.92	0.51
3:A:251:LEU:O	3:A:255:ARG:HG3	2.10	0.51
3:A:427:ILE:CG2	3:A:427:ILE:O	2.54	0.51
3:A:387:ALA:HB3	3:A:390:THR:HG21	1.93	0.51
3:A:220:PHE:HB3	3:A:422:TRP:CH2	2.46	0.51
3:A:555:VAL:HG11	3:A:646:ASP:OD2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:289:TYR:HB3	3:A:299:ARG:HG2	1.93	0.51
3:A:568:LEU:CD2	3:A:568:LEU:C	2.79	0.51
5:E:1297:ARG:NH1	5:E:1297:ARG:HB3	2.24	0.51
4:D:104:THR:HA	4:D:107:GLU:HB3	1.92	0.50
3:A:571:ASP:OD2	5:E:1136:ALA:HB1	2.11	0.50
5:E:1178:GLN:O	5:E:1180:ALA:N	2.44	0.50
3:A:349:TYR:HB2	3:A:353:MET:HB3	1.93	0.50
3:A:644:ARG:C	3:A:646:ASP:H	2.13	0.50
3:A:402:THR:HG23	3:A:403:VAL:N	2.27	0.50
3:A:619:VAL:HG11	3:A:638:VAL:HG11	1.94	0.50
5:E:1159:LEU:N	5:E:1159:LEU:HD13	2.27	0.50
1:B:13:DA:H2''	1:B:14:DG:H5''	1.93	0.50
5:E:1141:GLY:O	5:E:1144:VAL:HG12	2.11	0.50
5:E:1252:GLY:HA3	5:E:1286:HIS:CE1	2.46	0.50
3:A:386:ILE:HD13	3:A:392:VAL:HG11	1.94	0.50
4:D:66:GLY:O	4:D:68:GLU:N	2.44	0.50
5:E:935:ARG:HB2	5:E:1199:ARG:NH2	2.27	0.50
3:A:243:TYR:CB	3:A:245:ILE:HD11	2.41	0.50
3:A:474:VAL:HG21	3:A:535:ALA:HB1	1.93	0.50
5:E:1220:MSE:HE1	5:E:1259:TYR:CD1	2.46	0.50
5:E:1276:THR:C	5:E:1280:LEU:HD23	2.32	0.50
5:E:1276:THR:HG22	5:E:1279:GLN:NE2	2.17	0.50
5:E:1184:LEU:HD13	5:E:1188:LYS:HG2	1.92	0.50
3:A:568:LEU:HB2	3:A:654:LEU:HD23	1.94	0.50
3:A:659:LYS:HD3	5:E:1052:HIS:HD2	1.77	0.50
5:E:1022:SER:O	5:E:1023:PRO:C	2.51	0.49
5:E:1028:THR:HG23	5:E:1029:GLU:N	2.27	0.49
2:C:1:DA:H1'	2:C:2:DA:H5'	1.94	0.49
5:E:1099:MSE:C	5:E:1101:ALA:N	2.64	0.49
5:E:1138:ARG:CG	5:E:1178:GLN:HE22	2.23	0.49
3:A:608:SER:O	3:A:609:LEU:HD23	2.12	0.49
1:B:6:DG:H4'	3:A:235:PHE:CE2	2.45	0.49
5:E:1086:ASP:C	5:E:1088:ASN:N	2.66	0.49
4:D:86:PRO:HA	4:D:89:ILE:CG1	2.39	0.49
5:E:1072:LEU:HD13	5:E:1076:GLU:OE2	2.12	0.49
5:E:1099:MSE:O	5:E:1101:ALA:N	2.45	0.49
3:A:319:PRO:HG2	3:A:321:ILE:HG13	1.94	0.49
3:A:560:SER:O	3:A:562:CYS:N	2.46	0.49
3:A:637:GLU:HG3	3:A:637:GLU:O	2.13	0.49
5:E:1056:VAL:CG1	5:E:1060:ILE:HD11	2.42	0.49
5:E:1081:ILE:HD13	5:E:1082:ALA:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1153:LYS:HA	5:E:1156:ILE:HG12	1.94	0.49
5:E:1252:GLY:HA3	5:E:1286:HIS:ND1	2.28	0.49
3:A:245:ILE:HG22	3:A:246:GLY:N	2.27	0.49
5:E:1201:ASP:OD1	5:E:1202:SER:N	2.42	0.49
3:A:394:LEU:HD11	3:A:457:LEU:HD13	1.94	0.49
3:A:506:VAL:HG13	3:A:518:HIS:H	1.76	0.49
3:A:388:SER:CB	5:E:1202:SER:OG	2.56	0.49
5:E:1110:VAL:CG2	5:E:1142:MSE:HE1	2.36	0.49
3:A:220:PHE:CE2	3:A:543:LYS:HD2	2.48	0.48
3:A:224:VAL:HG11	3:A:492:GLN:HG2	1.94	0.48
2:C:1:DA:H1'	2:C:2:DA:C5'	2.43	0.48
5:E:1114:MSE:HA	5:E:1118:ALA:HB3	1.95	0.48
5:E:1233:ASN:C	5:E:1235:ASP:H	2.16	0.48
5:E:1253:ARG:O	5:E:1256:VAL:HG12	2.13	0.48
5:E:1133:GLN:CA	5:E:1133:GLN:NE2	2.74	0.48
5:E:1220:MSE:HB2	5:E:1221:PRO:HD3	1.94	0.48
3:A:215:CYS:HB2	3:A:548:PHE:O	2.13	0.48
3:A:432:ASP:O	3:A:433:GLU:HB2	2.12	0.48
3:A:462:THR:OG1	3:A:463:GLY:N	2.46	0.48
5:E:1064:SER:C	5:E:1066:ALA:N	2.67	0.48
2:C:14:DG:H2''	2:C:15:DT:O5'	2.12	0.48
4:D:76:LEU:C	4:D:76:LEU:HD13	2.33	0.48
4:D:83:LYS:CD	4:D:84:ALA:N	2.75	0.48
3:A:516:ILE:HA	5:E:947:PRO:HB2	1.96	0.48
3:A:223:LYS:HD2	3:A:383:TYR:CE2	2.40	0.48
3:A:593:TRP:CE2	3:A:598:PRO:HB3	2.48	0.48
5:E:1058:HIS:CE1	5:E:1089:ALA:O	2.66	0.48
5:E:1201:ASP:O	5:E:1202:SER:O	2.31	0.48
5:E:1219:ASN:O	5:E:1220:MSE:C	2.52	0.48
4:D:91:ASN:ND2	4:D:91:ASN:H	2.12	0.48
5:E:1099:MSE:HE1	5:E:1130:ALA:CA	2.38	0.48
3:A:472:ARG:O	3:A:496:CYS:HB2	2.13	0.48
5:E:1173:ASN:O	5:E:1178:GLN:HG2	2.14	0.48
3:A:604:ARG:NH2	3:A:604:ARG:HG2	2.25	0.48
3:A:613:ILE:N	3:A:613:ILE:HD12	2.29	0.48
5:E:1253:ARG:HA	5:E:1253:ARG:NE	2.29	0.48
3:A:242:ILE:N	3:A:242:ILE:HD12	2.28	0.48
3:A:250:LYS:O	3:A:253:LYS:HB3	2.14	0.48
3:A:310:ARG:HG2	3:A:310:ARG:HH11	1.79	0.48
3:A:548:PHE:C	3:A:548:PHE:CD2	2.86	0.48
4:D:91:ASN:ND2	4:D:91:ASN:N	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:935:ARG:HB2	5:E:1199:ARG:HH22	1.79	0.48
3:A:300:GLN:H	3:A:300:GLN:HE21	1.62	0.47
5:E:1242:LYS:HG2	5:E:1246:MSE:CE	2.44	0.47
3:A:411:GLU:O	3:A:412:GLY:C	2.50	0.47
3:A:506:VAL:HG11	3:A:517:GLN:HE21	1.80	0.47
5:E:935:ARG:NH1	5:E:1158:GLU:CG	2.59	0.47
3:A:441:ASN:HA	5:E:941:ASN:HA	1.96	0.47
5:E:1022:SER:N	5:E:1023:PRO:CD	2.73	0.47
5:E:1040:ILE:N	5:E:1040:ILE:CD1	2.77	0.47
5:E:1087:VAL:CG2	5:E:1118:ALA:HB2	2.44	0.47
5:E:1167:LEU:CD1	5:E:1167:LEU:N	2.65	0.47
5:E:1182:ALA:C	5:E:1184:LEU:N	2.67	0.47
3:A:199:THR:O	3:A:200:SER:C	2.52	0.47
3:A:418:SER:HB3	3:A:421:LYS:O	2.15	0.47
3:A:451:TYR:CE1	3:A:490:VAL:HG22	2.50	0.47
3:A:508:LEU:HD11	3:A:515:ILE:CG2	2.45	0.47
1:B:13:DA:C1'	1:B:14:DG:H5''	2.42	0.47
4:D:64:HIS:C	4:D:66:GLY:N	2.68	0.47
4:D:80:ASN:O	4:D:83:LYS:HB3	2.13	0.47
5:E:1252:GLY:HA2	5:E:1289:ILE:HD11	1.96	0.47
3:A:550:GLU:HA	3:A:648:VAL:HG23	1.97	0.47
3:A:254:ASP:C	3:A:256:VAL:H	2.17	0.47
5:E:1093:ASP:HA	5:E:1125:LYS:HD2	1.97	0.47
1:B:13:DA:H2''	1:B:14:DG:C5'	2.45	0.47
5:E:1034:TYR:HD1	5:E:1035:ALA:N	1.94	0.47
5:E:1045:VAL:HG12	5:E:1056:VAL:CG2	2.41	0.47
5:E:1243:THR:O	5:E:1244:PRO:C	2.53	0.47
5:E:1276:THR:O	5:E:1278:ARG:N	2.48	0.47
5:E:1196:GLY:O	5:E:1199:ARG:N	2.47	0.47
5:E:1208:ARG:HB3	5:E:1212:HIS:HB2	1.96	0.47
3:A:254:ASP:O	3:A:256:VAL:N	2.47	0.47
3:A:560:SER:CB	3:A:561:PRO:CD	2.90	0.47
4:D:76:LEU:O	4:D:76:LEU:HD22	2.14	0.47
5:E:1180:ALA:C	5:E:1182:ALA:N	2.67	0.47
3:A:415:PHE:CZ	3:A:466:LEU:HG	2.50	0.46
3:A:493:LEU:CD2	3:A:539:ILE:HD12	2.41	0.46
5:E:1073:ILE:HD11	5:E:1106:ARG:NH2	2.30	0.46
5:E:1220:MSE:HE1	5:E:1259:TYR:HD1	1.80	0.46
3:A:555:VAL:HG12	3:A:556:ALA:N	2.31	0.46
5:E:1099:MSE:CE	5:E:1130:ALA:HA	2.40	0.46
3:A:362:ARG:H	3:A:362:ARG:HD2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:510:LEU:HG	3:A:510:LEU:O	2.15	0.46
3:A:569:GLU:CG	5:E:1128:ARG:NH2	2.78	0.46
5:E:1199:ARG:NH1	5:E:1203:GLU:OE1	2.48	0.46
5:E:1234:LYS:HG3	5:E:1265:ALA:HB2	1.98	0.46
3:A:441:ASN:HB2	5:E:939:MSE:CE	2.46	0.46
3:A:406:ARG:CZ	3:A:419:SER:HB3	2.45	0.46
3:A:508:LEU:HD11	3:A:515:ILE:HG21	1.96	0.46
5:E:1097:PRO:HA	5:E:1100:LEU:HD13	1.98	0.46
5:E:1259:TYR:CE2	5:E:1263:GLN:HG3	2.50	0.46
5:E:943:SER:OG	5:E:944:VAL:N	2.46	0.46
5:E:1107:ARG:HA	5:E:1142:MSE:HE1	1.96	0.46
5:E:1121:THR:O	5:E:1122:ILE:C	2.53	0.46
3:A:255:ARG:HH21	3:A:553:GLY:HA2	1.80	0.46
3:A:265:ALA:O	3:A:266:SER:HB3	2.15	0.46
3:A:506:VAL:CG1	3:A:517:GLN:HG2	2.46	0.46
3:A:254:ASP:C	3:A:256:VAL:N	2.69	0.46
3:A:342:ASP:OD1	3:A:342:ASP:N	2.45	0.46
3:A:568:LEU:C	3:A:569:GLU:OE1	2.54	0.46
3:A:616:VAL:HG22	3:A:658:TYR:CE1	2.50	0.46
3:A:215:CYS:HB3	3:A:548:PHE:CE2	2.50	0.46
3:A:523:ILE:HG23	3:A:524:ASN:N	2.30	0.46
5:E:1029:GLU:O	5:E:1030:ALA:C	2.54	0.46
5:E:1066:ALA:O	5:E:1067:GLU:CB	2.63	0.46
5:E:1193:ASP:OD1	5:E:1232:SER:HA	2.15	0.46
3:A:290:ILE:CD1	3:A:345:ALA:HB2	2.45	0.46
3:A:568:LEU:HD23	3:A:569:GLU:N	2.30	0.46
5:E:1174:GLU:CG	5:E:1175:GLY:H	2.29	0.46
3:A:258:GLN:HA	3:A:261:LYS:HE2	1.97	0.46
3:A:514:LYS:HA	3:A:514:LYS:HD3	1.76	0.46
3:A:563:PRO:HG3	3:A:650:TYR:CD2	2.51	0.46
3:A:620:ARG:HA	3:A:624:THR:OG1	2.15	0.46
5:E:1025:LYS:O	5:E:1029:GLU:HG3	2.16	0.46
5:E:1113:LEU:HD13	5:E:1113:LEU:HA	1.73	0.46
3:A:447:GLY:HA2	5:E:1201:ASP:OD1	2.16	0.45
3:A:510:LEU:HD23	3:A:510:LEU:H	1.81	0.45
5:E:1064:SER:O	5:E:1066:ALA:N	2.40	0.45
5:E:1133:GLN:O	5:E:1137:ASN:OD1	2.34	0.45
3:A:431:ASP:HB3	3:A:443:ALA:CB	2.45	0.45
3:A:470:ARG:HB3	3:A:499:GLN:HG2	1.98	0.45
3:A:542:ASP:CG	3:A:543:LYS:N	2.69	0.45
1:B:7:DT:H2"	1:B:8:DG:H8	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1056:VAL:C	5:E:1060:ILE:HG12	2.36	0.45
5:E:1087:VAL:CG2	5:E:1113:LEU:HD12	2.46	0.45
5:E:933:ARG:NH1	5:E:1090:MSE:SE	2.88	0.45
5:E:1140:PHE:C	5:E:1140:PHE:HD1	2.17	0.45
5:E:1291:ASP:O	5:E:1295:ARG:HB2	2.16	0.45
3:A:255:ARG:HH21	3:A:553:GLY:CA	2.28	0.45
5:E:1183:LYS:O	5:E:1186:VAL:HG13	2.17	0.45
5:E:1218:SER:N	5:E:1253:ARG:HG3	2.27	0.45
3:A:280:GLU:C	3:A:282:GLN:H	2.20	0.45
5:E:1199:ARG:O	5:E:1201:ASP:N	2.49	0.45
5:E:1289:ILE:O	5:E:1290:VAL:C	2.53	0.45
3:A:499:GLN:HA	3:A:506:VAL:O	2.17	0.45
5:E:1063:ASN:C	5:E:1065:SER:H	2.20	0.45
5:E:1273:THR:O	5:E:1275:HIS:HD2	2.00	0.45
3:A:593:TRP:NE1	3:A:598:PRO:HB3	2.32	0.45
4:D:113:GLU:O	4:D:114:GLN:HG3	2.17	0.45
5:E:1178:GLN:C	5:E:1180:ALA:H	2.20	0.45
3:A:588:PRO:HG3	3:A:603:PHE:CD1	2.52	0.45
5:E:1026:LEU:O	5:E:1029:GLU:HB2	2.17	0.45
5:E:1174:GLU:HG2	5:E:1175:GLY:H	1.80	0.45
5:E:1219:ASN:C	5:E:1221:PRO:HD2	2.36	0.45
3:A:245:ILE:N	3:A:245:ILE:CD1	2.80	0.45
3:A:394:LEU:HD11	3:A:457:LEU:CD1	2.46	0.45
5:E:1098:LEU:HD11	5:E:1146:MSE:CE	2.47	0.45
5:E:1133:GLN:O	5:E:1134:ALA:C	2.55	0.45
3:A:430:PHE:HB3	3:A:454:VAL:HB	1.98	0.45
5:E:1089:ALA:O	5:E:1097:PRO:HD3	2.16	0.45
5:E:1179:VAL:HG22	5:E:1179:VAL:O	2.17	0.45
3:A:557:ASN:HB3	3:A:558:PRO:CD	2.47	0.45
3:A:616:VAL:HG22	3:A:658:TYR:CD1	2.52	0.45
5:E:1026:LEU:HD12	5:E:1026:LEU:C	2.37	0.45
5:E:1034:TYR:CD1	5:E:1035:ALA:N	2.75	0.45
5:E:1073:ILE:HD11	5:E:1106:ARG:NH1	2.31	0.45
5:E:1209:THR:N	5:E:1212:HIS:ND1	2.65	0.45
5:E:1234:LYS:CD	5:E:1234:LYS:H	2.25	0.44
2:C:12:DC:H2''	2:C:13:DA:C8	2.53	0.44
5:E:1029:GLU:OE1	5:E:1037:THR:HB	2.17	0.44
5:E:1141:GLY:O	5:E:1142:MSE:C	2.55	0.44
5:E:1244:PRO:O	5:E:1245:ILE:C	2.55	0.44
3:A:244:LEU:HD23	3:A:244:LEU:HA	1.83	0.44
1:B:8:DG:OP1	3:A:397:ARG:HD3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:ILE:HD13	3:A:501:ILE:C	2.38	0.44
1:B:6:DG:H21	3:A:400:SER:HB3	1.82	0.44
3:A:515:ILE:HG22	3:A:516:ILE:N	2.31	0.44
3:A:605:SER:C	3:A:607:GLU:H	2.20	0.44
3:A:244:LEU:O	3:A:322:TYR:HB3	2.18	0.44
3:A:599:VAL:CG1	3:A:600:GLU:N	2.80	0.44
3:A:592:VAL:HA	3:A:641:SER:O	2.18	0.44
3:A:644:ARG:C	3:A:646:ASP:N	2.71	0.44
5:E:1233:ASN:C	5:E:1235:ASP:N	2.71	0.44
3:A:206:PHE:CE2	3:A:649:VAL:HG21	2.53	0.44
3:A:239:PRO:HA	3:A:240:PRO:HD3	1.88	0.44
3:A:328:LYS:H	3:A:328:LYS:CD	2.06	0.44
3:A:411:GLU:HG3	3:A:416:HIS:NE2	2.33	0.44
4:D:65:SER:O	4:D:68:GLU:HB2	2.17	0.44
5:E:1025:LYS:HD3	5:E:1038:GLU:OE1	2.17	0.44
5:E:1099:MSE:SE	5:E:1133:GLN:HG3	2.68	0.44
5:E:1200:LYS:C	5:E:1201:ASP:O	2.54	0.44
5:E:1207:GLY:HA2	5:E:1239:GLU:H	1.83	0.44
3:A:198:LEU:HD12	3:A:199:THR:N	2.33	0.43
4:D:85:ARG:N	4:D:86:PRO:HD2	2.33	0.43
3:A:573:HIS:O	3:A:575:GLU:N	2.51	0.43
3:A:398:LEU:N	3:A:398:LEU:HD22	2.32	0.43
3:A:589:ASN:HD22	4:D:81:TYR:HE2	1.65	0.43
3:A:416:HIS:CG	3:A:417:ALA:N	2.87	0.43
3:A:215:CYS:CB	3:A:548:PHE:HE2	2.31	0.43
3:A:252:LYS:HZ1	3:A:554:GLN:HB2	1.83	0.43
5:E:940:ILE:HG22	5:E:940:ILE:O	2.17	0.43
3:A:609:LEU:HD12	3:A:642:LEU:HD21	2.00	0.43
1:B:6:DG:H2'	1:B:7:DT:C7	2.48	0.43
4:D:76:LEU:O	4:D:79:ALA:HB3	2.19	0.43
3:A:451:TYR:CD1	3:A:490:VAL:HG22	2.54	0.43
1:B:6:DG:H2''	1:B:7:DT:C6	2.54	0.43
5:E:1025:LYS:O	5:E:1028:THR:HG22	2.18	0.43
5:E:1033:SER:O	5:E:1069:SER:CB	2.66	0.43
5:E:1178:GLN:C	5:E:1180:ALA:N	2.71	0.43
5:E:1243:THR:O	5:E:1246:MSE:N	2.51	0.43
3:A:235:PHE:CD1	3:A:329:THR:HA	2.53	0.43
5:E:1075:HIS:C	5:E:1077:ALA:N	2.71	0.43
5:E:1165:THR:OG1	5:E:1168:MSE:HE3	2.19	0.43
3:A:388:SER:HB2	3:A:447:GLY:N	2.33	0.43
3:A:430:PHE:C	3:A:430:PHE:CD1	2.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1243:THR:H	5:E:1246:MSE:SE	2.51	0.43
5:E:1253:ARG:HB2	5:E:1256:VAL:HG12	2.01	0.43
3:A:302:LEU:CD2	3:A:327:ALA:HB2	2.49	0.43
3:A:603:PHE:CE1	3:A:606:GLU:HA	2.54	0.43
2:C:13:DA:C4	2:C:14:DG:N7	2.87	0.43
5:E:1073:ILE:CD1	5:E:1106:ARG:CZ	2.86	0.43
5:E:1217:VAL:HG23	5:E:1251:GLU:CB	2.48	0.43
3:A:516:ILE:HG22	5:E:948:PRO:HG2	2.00	0.43
3:A:539:ILE:HG23	3:A:539:ILE:O	2.18	0.42
5:E:1072:LEU:C	5:E:1072:LEU:HD12	2.39	0.42
5:E:1219:ASN:O	5:E:1219:ASN:OD1	2.36	0.42
5:E:1278:ARG:O	5:E:1279:GLN:C	2.56	0.42
3:A:362:ARG:H	3:A:362:ARG:CD	2.32	0.42
3:A:530:ILE:N	3:A:530:ILE:CD1	2.81	0.42
5:E:1192:VAL:CG1	5:E:1226:LEU:HD22	2.50	0.42
3:A:341:PHE:CD1	3:A:341:PHE:C	2.92	0.42
3:A:196:GLN:HB3	3:A:552:MET:HG3	2.01	0.42
4:D:92:GLN:NE2	4:D:96:THR:HB	2.33	0.42
3:A:388:SER:OG	3:A:445:ARG:O	2.31	0.42
3:A:586:PHE:CE2	3:A:642:LEU:HD11	2.54	0.42
4:D:109:ARG:HA	4:D:112:VAL:HG22	2.01	0.42
5:E:1057:LEU:HA	5:E:1060:ILE:CG1	2.49	0.42
5:E:1066:ALA:C	5:E:1068:LYS:H	2.22	0.42
5:E:1063:ASN:HD21	5:E:1106:ARG:HH11	1.67	0.42
3:A:348:PHE:HA	3:A:355:ILE:HG12	2.02	0.42
3:A:427:ILE:HG13	3:A:457:LEU:CD2	2.49	0.42
3:A:215:CYS:CB	3:A:548:PHE:CE2	3.02	0.42
3:A:213:TYR:CB	3:A:549:PHE:CE2	2.99	0.42
3:A:597:THR:HA	3:A:598:PRO:HD2	1.85	0.42
3:A:648:VAL:O	3:A:648:VAL:CG1	2.68	0.42
3:A:251:LEU:HD13	3:A:251:LEU:C	2.40	0.42
3:A:388:SER:HB2	3:A:447:GLY:H	1.85	0.42
3:A:481:LEU:HD12	3:A:481:LEU:O	2.19	0.42
3:A:386:ILE:HD12	3:A:538:ILE:HD13	2.00	0.42
3:A:416:HIS:HD1	3:A:417:ALA:H	1.67	0.42
3:A:413:ASN:HA	3:A:464:ILE:HD12	2.00	0.42
5:E:1078:LYS:CA	5:E:1081:ILE:HG23	2.49	0.42
5:E:1182:ALA:O	5:E:1183:LYS:C	2.56	0.42
5:E:1188:LYS:HD3	5:E:1188:LYS:HA	1.68	0.42
5:E:1210:ALA:O	5:E:1211:LEU:C	2.58	0.42
3:A:252:LYS:HD2	3:A:252:LYS:HA	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1043:GLU:O	5:E:1048:ILE:HD13	2.20	0.42
3:A:485:CYS:C	3:A:487:GLU:H	2.23	0.42
5:E:1034:TYR:O	5:E:1036:ILE:HG13	2.20	0.42
5:E:1026:LEU:HD12	5:E:1026:LEU:O	2.20	0.42
5:E:1075:HIS:C	5:E:1077:ALA:H	2.24	0.42
5:E:1091:ASP:O	5:E:1092:CYS:C	2.58	0.42
5:E:1237:GLN:HB3	5:E:1241:GLY:CA	2.45	0.42
5:E:1253:ARG:CB	5:E:1256:VAL:HG12	2.50	0.42
3:A:407:TYR:CG	3:A:422:TRP:HB3	2.55	0.41
5:E:1059:TRP:O	5:E:1062:SER:HB3	2.19	0.41
5:E:1166:ALA:HB1	5:E:1185:LEU:CD1	2.50	0.41
5:E:1167:LEU:HA	5:E:1170:VAL:HB	2.00	0.41
5:E:1126:SER:O	5:E:1128:ARG:N	2.53	0.41
5:E:1182:ALA:O	5:E:1184:LEU:N	2.53	0.41
5:E:1078:LYS:CA	5:E:1081:ILE:CG2	2.96	0.41
5:E:1054:ARG:HG2	5:E:1091:ASP:HB3	2.01	0.41
5:E:1135:ALA:N	5:E:1143:MSE:HE2	2.35	0.41
4:D:53:ASP:OD1	5:E:1108:ARG:NH2	2.53	0.41
3:A:659:LYS:CD	5:E:1052:HIS:HD2	2.33	0.41
5:E:1053:ASN:O	5:E:1091:ASP:HA	2.21	0.41
5:E:935:ARG:HB3	5:E:1199:ARG:HH22	1.84	0.41
3:A:249:TRP:HB3	3:A:322:TYR:CE1	2.56	0.41
3:A:388:SER:HB3	5:E:1202:SER:CB	2.48	0.41
3:A:408:LEU:HD22	3:A:425:PHE:CE1	2.55	0.41
3:A:553:GLY:O	3:A:554:GLN:C	2.58	0.41
3:A:614:PRO:HA	3:A:615:PRO:HD3	1.91	0.41
5:E:1254:ILE:HG13	5:E:1255:GLU:N	2.36	0.41
3:A:217:ILE:O	3:A:217:ILE:HG23	2.21	0.41
3:A:642:LEU:HA	3:A:642:LEU:HD23	1.82	0.41
5:E:1233:ASN:O	5:E:1235:ASP:N	2.54	0.41
3:A:249:TRP:HB3	3:A:322:TYR:CD1	2.55	0.41
3:A:287:VAL:CB	3:A:348:PHE:CE1	3.04	0.41
3:A:559:ILE:O	3:A:561:PRO:N	2.53	0.41
5:E:1140:PHE:HD1	5:E:1141:GLY:N	2.19	0.41
3:A:348:PHE:C	3:A:348:PHE:CD1	2.93	0.41
3:A:348:PHE:HB2	3:A:353:MET:O	2.21	0.41
3:A:446:ASP:OD2	5:E:1203:GLU:HG3	2.21	0.41
3:A:442:PHE:CZ	3:A:456:LYS:HE2	2.56	0.41
1:B:6:DG:H2''	1:B:7:DT:H6	1.86	0.41
2:C:1:DA:H1'	2:C:2:DA:O5'	2.21	0.41
5:E:1040:ILE:HG22	5:E:1040:ILE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1253:ARG:O	5:E:1257:VAL:HG23	2.20	0.41
5:E:1271:ASP:OD2	5:E:1275:HIS:HB2	2.21	0.41
3:A:441:ASN:HB3	5:E:941:ASN:HB3	2.02	0.41
3:A:466:LEU:HB3	3:A:467:PRO:HD2	2.03	0.41
3:A:255:ARG:NH2	3:A:553:GLY:HA2	2.36	0.41
3:A:654:LEU:HD12	3:A:654:LEU:HA	1.86	0.41
5:E:1028:THR:O	5:E:1032:GLY:N	2.38	0.41
5:E:1033:SER:O	5:E:1069:SER:HB3	2.20	0.41
5:E:1048:ILE:N	5:E:1048:ILE:CD1	2.83	0.41
5:E:1216:GLN:O	5:E:1217:VAL:O	2.39	0.41
3:A:475:ASP:O	3:A:476:LYS:C	2.59	0.40
3:A:610:HIS:HE1	5:E:1173:ASN:HD21	1.68	0.40
3:A:220:PHE:CD2	3:A:220:PHE:N	2.90	0.40
3:A:280:GLU:C	3:A:282:GLN:N	2.74	0.40
3:A:343:LEU:O	3:A:359:VAL:HA	2.21	0.40
3:A:399:ARG:O	3:A:401:GLN:N	2.55	0.40
4:D:57:ILE:HB	4:D:58:GLY:H	1.58	0.40
5:E:1061:ALA:HA	5:E:1109:LEU:HD21	2.04	0.40
5:E:1225:TYR:OH	5:E:1229:GLU:OE1	2.37	0.40
3:A:340:TYR:CE2	3:A:383:TYR:CE1	3.10	0.40
3:A:409:HIS:ND1	3:A:410:VAL:N	2.69	0.40
3:A:602:THR:HG23	4:D:74:SER:HB2	2.02	0.40
4:D:90:ALA:C	4:D:92:GLN:N	2.74	0.40
3:A:416:HIS:ND1	3:A:417:ALA:N	2.70	0.40
5:E:1238:ASP:C	5:E:1240:ASP:H	2.25	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
3	A	429/477 (90%)	324 (76%)	77 (18%)	28 (6%)	1 7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	61/85 (72%)	44 (72%)	14 (23%)	3 (5%)	2	13
5	E	293/373 (79%)	170 (58%)	76 (26%)	47 (16%)	0	0
All	All	783/935 (84%)	538 (69%)	167 (21%)	78 (10%)	0	3

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	299	ARG
3	A	399	ARG
3	A	400	SER
3	A	403	VAL
3	A	504	GLU
3	A	513	ASP
3	A	553	GLY
3	A	560	SER
3	A	574	GLY
3	A	627	MET
3	A	634	GLY
4	D	55	PRO
4	D	59	ASP
5	E	943	SER
5	E	1023	PRO
5	E	1032	GLY
5	E	1045	VAL
5	E	1046	ASN
5	E	1062	SER
5	E	1066	ALA
5	E	1070	GLU
5	E	1122	ILE
5	E	1198	ALA
5	E	1201	ASP
5	E	1202	SER
5	E	1204	LYS
5	E	1206	LYS
5	E	1217	VAL
5	E	1218	SER
5	E	1219	ASN
5	E	1230	LYS
5	E	1277	ALA
3	A	266	SER
3	A	300	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	303	ASP
3	A	412	GLY
5	E	948	PRO
5	E	1022	SER
5	E	1050	PRO
5	E	1063	ASN
5	E	1087	VAL
5	E	1121	THR
5	E	1138	ARG
5	E	1203	GLU
5	E	1232	SER
5	E	1271	ASP
3	A	265	ALA
3	A	416	HIS
3	A	645	ASP
5	E	1024	ILE
5	E	1078	LYS
5	E	1140	PHE
5	E	1160	ASP
5	E	1166	ALA
5	E	1189	GLY
5	E	1210	ALA
3	A	207	LEU
3	A	214	GLU
3	A	255	ARG
3	A	479	VAL
3	A	532	ASP
5	E	1107	ARG
5	E	1127	GLU
5	E	1179	VAL
5	E	1234	LYS
5	E	1029	GLU
5	E	1068	LYS
5	E	1178	GLN
5	E	1208	ARG
5	E	1220	MSE
3	A	476	LYS
3	A	480	ILE
5	E	1120	PRO
5	E	1290	VAL
3	A	464	ILE
3	A	293	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	558	PRO
4	D	57	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	385/416 (92%)	341 (89%)	44 (11%)	5	23
4	D	54/73 (74%)	47 (87%)	7 (13%)	4	18
5	E	244/298 (82%)	210 (86%)	34 (14%)	3	15
All	All	683/787 (87%)	598 (88%)	85 (12%)	4	19

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	199	THR
3	A	202	ARG
3	A	217	ILE
3	A	239	PRO
3	A	249	TRP
3	A	256	VAL
3	A	258	GLN
3	A	296	THR
3	A	300	GLN
3	A	310	ARG
3	A	328	LYS
3	A	346	GLN
3	A	362	ARG
3	A	383	TYR
3	A	408	LEU
3	A	426	THR
3	A	441	ASN
3	A	454	VAL
3	A	464	ILE
3	A	472	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	482	ASP
3	A	485	CYS
3	A	492	GLN
3	A	501	ILE
3	A	503	ASN
3	A	511	SER
3	A	530	ILE
3	A	536	TRP
3	A	548	PHE
3	A	552	MET
3	A	559	ILE
3	A	569	GLU
3	A	570	VAL
3	A	571	ASP
3	A	592	VAL
3	A	620	ARG
3	A	623	GLN
3	A	630	ASN
3	A	631	ARG
3	A	644	ARG
3	A	648	VAL
3	A	651	SER
3	A	660	SER
3	A	662	GLU
4	D	55	PRO
4	D	75	GLU
4	D	76	LEU
4	D	91	ASN
4	D	93	ARG
4	D	102	ARG
4	D	109	ARG
5	E	937	ARG
5	E	1026	LEU
5	E	1034	TYR
5	E	1046	ASN
5	E	1055	THR
5	E	1057	LEU
5	E	1073	ILE
5	E	1079	GLU
5	E	1080	CYS
5	E	1081	ILE
5	E	1098	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	1105	ARG
5	E	1113	LEU
5	E	1126	SER
5	E	1137	ASN
5	E	1138	ARG
5	E	1140	PHE
5	E	1147	LEU
5	E	1153	LYS
5	E	1155	ASP
5	E	1159	LEU
5	E	1167	LEU
5	E	1168	MSE
5	E	1176	ARG
5	E	1178	GLN
5	E	1186	VAL
5	E	1202	SER
5	E	1229	GLU
5	E	1232	SER
5	E	1234	LYS
5	E	1243	THR
5	E	1244	PRO
5	E	1245	ILE
5	E	1288	ASN

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

Mol	Chain	Res	Type
3	A	221	HIS
3	A	258	GLN
3	A	301	GLN
3	A	320	ASN
3	A	361	GLN
3	A	401	GLN
3	A	478	GLN
3	A	503	ASN
3	A	517	GLN
3	A	519	GLN
3	A	524	ASN
3	A	528	HIS
3	A	557	ASN
3	A	610	HIS
3	A	630	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	70	HIS
4	D	80	ASN
4	D	91	ASN
4	D	92	GLN
4	D	114	GLN
5	E	1027	HIS
5	E	1046	ASN
5	E	1053	ASN
5	E	1058	HIS
5	E	1063	ASN
5	E	1132	HIS
5	E	1133	GLN
5	E	1137	ASN
5	E	1162	ASN
5	E	1172	HIS
5	E	1250	GLN
5	E	1263	GLN
5	E	1275	HIS
5	E	1279	GLN
5	E	1285	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	B	15/15 (100%)	-0.34	0	100	100	72, 88, 113, 115	0
2	C	15/15 (100%)	-0.38	0	100	100	66, 85, 113, 113	0
3	A	439/477 (92%)	0.03	17 (3%)	39	20	37, 97, 165, 197	0
4	D	63/85 (74%)	-0.50	0	100	100	68, 123, 174, 200	0
5	E	283/373 (75%)	-0.22	7 (2%)	57	35	52, 94, 165, 202	0
All	All	815/965 (84%)	-0.11	24 (2%)	51	29	37, 98, 166, 202	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	400	SER	8.0
3	A	484	SER	5.3
5	E	1203	GLU	4.2
3	A	626	TRP	3.6
3	A	661	LEU	3.6
3	A	399	ARG	3.5
5	E	1047	ILE	3.4
3	A	401	GLN	3.1
3	A	583	GLY	3.0
5	E	1021	GLU	2.9
3	A	195	VAL	2.8
3	A	196	GLN	2.8
5	E	1289	ILE	2.8
3	A	662	GLU	2.8
3	A	629	THR	2.7
3	A	266	SER	2.7
5	E	1260	LEU	2.5
3	A	663	ARG	2.5
3	A	623	GLN	2.4
5	E	952	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	482	ASP	2.3
5	E	1293	PHE	2.2
3	A	281	GLN	2.2
3	A	357	GLY	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.