



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:23 AM UTC

PDB ID : 5IUD / pdb_00005iud
Title : Human DNA polymerase alpha in binary complex with a DNA:DNA template-primer
Authors : Coloma, J.; Aggarwal, A.K.
Deposited on : 2016-03-17
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

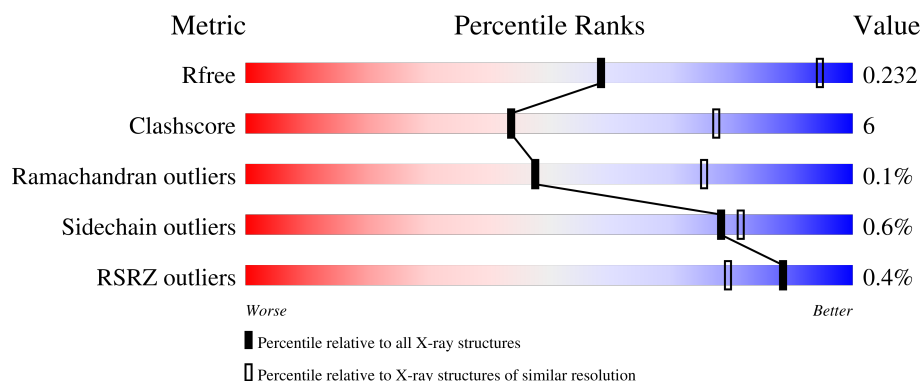
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	918	% 80% 14% 6%
1	D	918	82% 13% 5%
1	G	918	78% 16% 6%
1	J	918	80% 14% 6%
2	B	16	56% 38% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	16	 62% 38%
2	H	16	 56% 25% 19%
2	K	16	 56% 38% 6%
3	C	13	 85% 15%
3	F	13	 85% 15%
3	I	13	 77% 23%
3	L	13	 77% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28207 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 DNA polymerase alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	859	Total	C	N	O	S	0	0	0
			6480	4177	1082	1182	39			
1	D	871	Total	C	N	O	S	0	0	0
			6580	4231	1103	1206	40			
1	G	863	Total	C	N	O	S	0	0	0
			6456	4151	1075	1189	41			
1	J	861	Total	C	N	O	S	0	0	0
			6391	4110	1079	1165	37			

- Molecule 2 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			320	150	66	89	15			
2	E	16	Total	C	N	O	P	0	0	0
			341	160	71	94	16			
2	H	13	Total	C	N	O	P	0	0	0
			275	130	59	74	12			
2	K	15	Total	C	N	O	P	0	0	0
			317	150	66	87	14			

- Molecule 3 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	0
			251	123	39	77	12			
3	F	13	Total	C	N	O	P	0	0	0
			251	123	39	77	12			
3	I	10	Total	C	N	O	P	0	0	0
			194	94	29	61	10			
3	L	13	Total	C	N	O	P	0	0	0
			251	123	39	77	12			

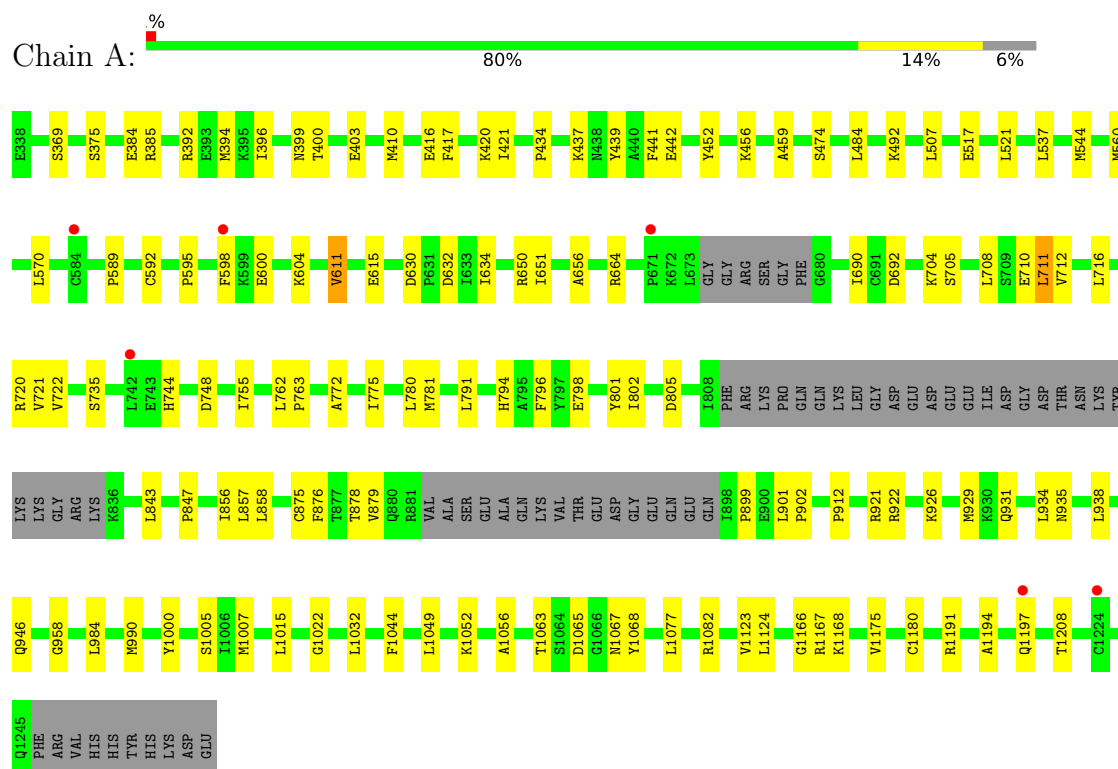
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total 31	O 31	0	0
4	B	2	Total 2	O 2	0	0
4	D	35	Total 35	O 35	0	0
4	E	3	Total 3	O 3	0	0
4	G	16	Total 16	O 16	0	0
4	H	1	Total 1	O 1	0	0
4	J	11	Total 11	O 11	0	0
4	L	1	Total 1	O 1	0	0

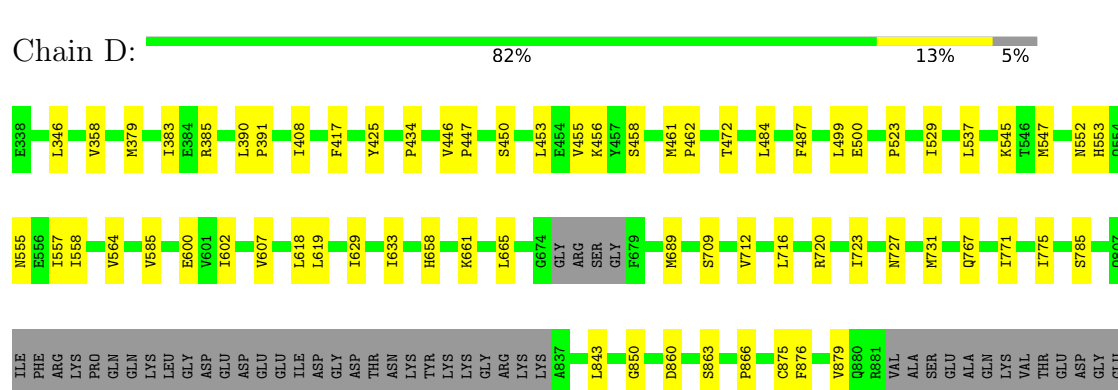
3 Residue-property plots [i](#)

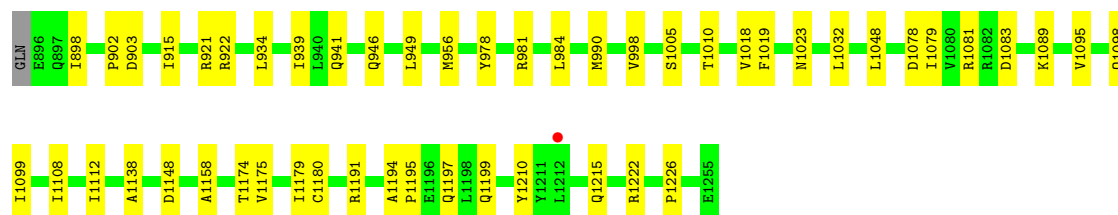
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA polymerase alpha catalytic subunit



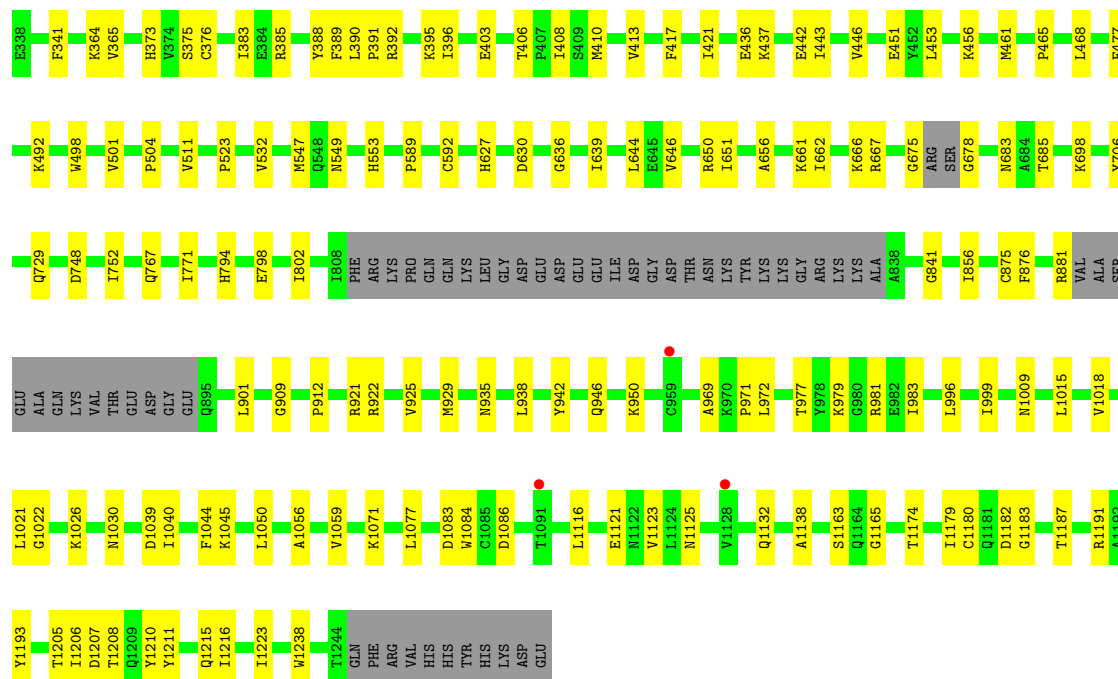
- Molecule 1: DNA polymerase alpha catalytic subunit





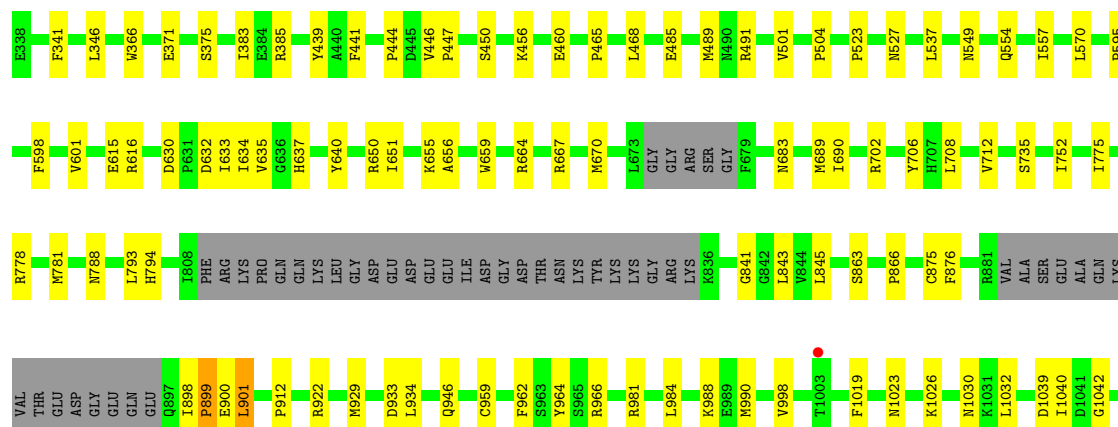
• Molecule 1: DNA polymerase alpha catalytic subunit

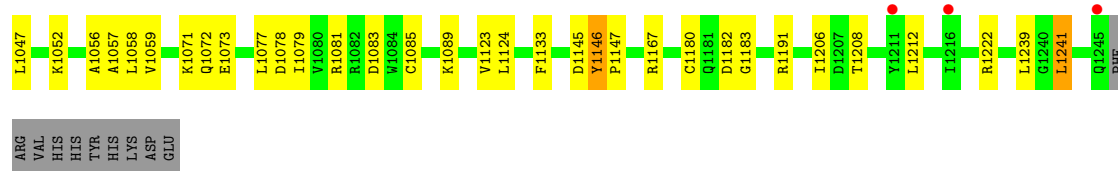
Chain G: 78% 16% 6%



• Molecule 1: DNA polymerase alpha catalytic subunit

Chain J: 80% 14% 6%





- Molecule 2: DNA template



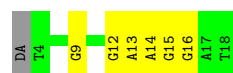
- Molecule 2: DNA template



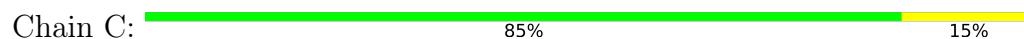
- Molecule 2: DNA template



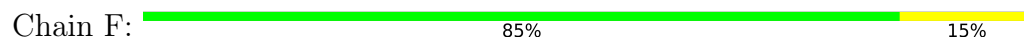
- Molecule 2: DNA template



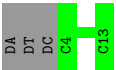
- Molecule 3: DNA primer



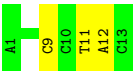
- Molecule 3: DNA primer



- Molecule 3: DNA primer



● Molecule 3: DNA primer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.04Å 132.03Å 163.14Å 90.00° 109.13° 90.00°	Depositor
Resolution (Å)	64.74 – 3.30 64.74 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (64.74-3.30) 93.4 (64.74-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.228 0.188 , 0.232	Depositor DCC
R_{free} test set	4123 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	86.1	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 99.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28207	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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	A	0.09	0/6620	0.26	0/9032
1	D	0.09	0/6726	0.25	0/9177
1	G	0.10	0/6595	0.27	0/9000
1	J	0.12	0/6527	0.28	0/8908
2	B	0.20	0/361	0.35	0/558
2	E	0.18	0/385	0.35	0/595
2	H	0.18	0/311	0.33	0/481
2	K	0.18	0/358	0.36	0/554
3	C	0.24	0/278	0.43	0/424
3	F	0.21	0/278	0.40	0/424
3	I	0.18	0/214	0.35	0/325
3	L	0.28	0/278	0.46	0/424
All	All	0.12	0/28931	0.28	0/39902

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6480	0	6180	76	0
1	D	6580	0	6225	69	0
1	G	6456	0	6089	87	0
1	J	6391	0	5989	83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	320	0	169	5	0
2	E	341	0	180	6	0
2	H	275	0	147	2	0
2	K	317	0	170	5	0
3	C	251	0	147	1	0
3	F	251	0	147	1	0
3	I	194	0	112	0	0
3	L	251	0	147	4	0
4	A	31	0	0	3	0
4	B	2	0	0	0	0
4	D	35	0	0	0	0
4	E	3	0	0	0	0
4	G	16	0	0	2	0
4	H	1	0	0	0	0
4	J	11	0	0	1	0
4	L	1	0	0	0	0
All	All	28207	0	25702	327	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 6.

All (327) 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:G:396:ILE:HG13	1:G:403:GLU:HB3	1.58	0.85
1:G:395:LYS:HB2	1:G:408:ILE:HD11	1.61	0.81
1:J:1146:TYR:OH	3:L:9:DC:OP1	2.06	0.71
1:G:1180:CYS:O	1:G:1191:ARG:NH1	2.25	0.69
1:G:1086:ASP:HB3	1:G:1132:GLN:HA	1.75	0.68
1:G:385:ARG:NH1	1:G:461:MET:O	2.27	0.68
1:G:1056:ALA:HB2	1:G:1077:LEU:HD11	1.75	0.68
1:G:364:LYS:HD2	1:G:373:HIS:HB3	1.76	0.67
1:G:875:CYS:HB2	1:G:912:PRO:HD3	1.77	0.67
1:D:1078:ASP:OD2	1:D:1222:ARG:NH1	2.28	0.67
1:J:1145:ASP:C	1:J:1147:PRO:HD3	2.21	0.66
1:A:1063:THR:HG23	1:A:1065:ASP:H	1.61	0.66
1:G:341:PHE:HB2	1:G:504:PRO:HG3	1.77	0.66
1:J:630:ASP:OD1	1:J:664:ARG:NH1	2.29	0.65
1:G:465:PRO:HG2	1:G:468:LEU:HB2	1.79	0.65
1:A:856:ILE:HB	1:A:1044:PHE:HB2	1.78	0.65
1:A:1166:GLY:O	1:A:1168:LYS:NZ	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:ARG:NH2	1:D:461:MET:O	2.30	0.64
1:J:1026:LYS:O	1:J:1030:ASN:ND2	2.29	0.64
1:D:447:PRO:HG2	1:D:450:SER:HB2	1.80	0.64
1:J:1146:TYR:OH	3:L:9:DC:P	2.56	0.64
1:A:1180:CYS:O	1:A:1191:ARG:NH1	2.31	0.64
1:A:396:ILE:HG22	1:A:403:GLU:HA	1.78	0.63
1:G:547:MET:HE3	1:G:589:PRO:HG3	1.79	0.63
1:J:383:ILE:HG12	1:J:523:PRO:HG3	1.79	0.63
1:G:651:ILE:HG23	1:G:656:ALA:HB3	1.81	0.63
1:J:1123:VAL:HG12	1:J:1208:THR:HG23	1.80	0.63
1:J:1056:ALA:HB2	1:J:1077:LEU:HD11	1.81	0.62
1:G:392:ARG:HD3	1:G:396:ILE:HD13	1.81	0.62
1:A:589:PRO:HD2	1:A:592:CYS:HB2	1.82	0.62
1:D:934:LEU:HD23	1:D:939:ILE:HG12	1.80	0.62
1:J:651:ILE:HG23	1:J:656:ALA:HB3	1.82	0.62
1:D:564:VAL:HG21	1:D:629:ILE:HD13	1.81	0.61
1:D:922:ARG:NH1	1:D:946:GLN:OE1	2.33	0.61
1:A:990:MET:HE1	1:A:1032:LEU:HD11	1.81	0.61
1:A:875:CYS:HB2	1:A:912:PRO:HD3	1.83	0.61
1:A:721:VAL:O	1:A:744:HIS:NE2	2.34	0.60
1:D:1194:ALA:HB3	1:D:1197:GLN:HG3	1.82	0.60
1:J:667:ARG:NH1	1:J:683:ASN:O	2.29	0.60
1:A:507:LEU:HD12	1:A:517:GLU:HB3	1.82	0.60
1:A:600:GLU:O	1:A:604:LYS:N	2.33	0.60
1:G:396:ILE:HA	1:G:403:GLU:HA	1.81	0.60
1:A:1063:THR:HG23	1:A:1065:ASP:N	2.16	0.60
1:G:1116:LEU:HD23	1:G:1238:TRP:HE3	1.67	0.60
1:J:1058:LEU:HA	1:J:1072:GLN:HA	1.83	0.60
1:D:843:LEU:HB2	1:D:981:ARG:HG2	1.84	0.59
2:E:16:DG:H2''	2:E:17:DA:C8	2.37	0.59
1:D:408:ILE:HD12	1:D:472:THR:HG22	1.85	0.59
1:D:1222:ARG:NH2	2:E:12:DG:OP1	2.36	0.58
1:D:383:ILE:HG12	1:D:523:PRO:HG3	1.85	0.58
1:G:442:GLU:HG2	1:G:443:ILE:HG23	1.84	0.58
1:A:1167:ARG:NH1	4:A:1302:HOH:O	2.31	0.58
1:G:1191:ARG:NH1	1:G:1207:ASP:OD2	2.35	0.58
1:D:1010:THR:HG21	1:D:1018:VAL:HG13	1.85	0.58
1:J:465:PRO:HG2	1:J:468:LEU:HB2	1.85	0.58
1:G:1179:ILE:N	1:G:1211:TYR:OH	2.33	0.58
1:D:898:ILE:HD13	1:D:978:TYR:HB2	1.86	0.57
1:G:1121:GLU:O	1:G:1125:ASN:ND2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:VAL:HG13	1:A:716:LEU:HD12	1.86	0.57
1:J:447:PRO:HG2	1:J:450:SER:HB2	1.85	0.57
1:J:346:LEU:HB3	1:J:689:MET:HE3	1.87	0.57
1:J:557:ILE:N	1:J:615:GLU:OE2	2.36	0.57
1:A:958:GLY:HA3	2:B:5:DG:H8	1.70	0.57
1:J:1079:ILE:HG22	1:J:1089:LYS:HA	1.86	0.57
1:A:416:GLU:HG3	1:A:420:LYS:HE2	1.87	0.57
2:K:12:DG:H2'	2:K:13:DA:C8	2.40	0.57
1:A:484:LEU:HD21	1:A:775:ILE:HD11	1.87	0.56
1:J:845:LEU:HD13	1:J:988:LYS:HD3	1.87	0.56
1:A:392:ARG:HG3	1:A:474:SER:HB3	1.86	0.56
1:J:990:MET:HE1	1:J:1032:LEU:HD11	1.87	0.56
1:A:544:MET:HE2	1:A:560:MET:HE3	1.86	0.56
2:E:15:DG:H2''	2:E:16:DG:H5''	1.86	0.56
1:A:598:PHE:HE2	1:A:611:VAL:HG22	1.71	0.56
1:D:602:ILE:HG23	1:D:607:VAL:HG23	1.87	0.56
1:G:1138:ALA:HB2	1:G:1174:THR:HG22	1.87	0.55
1:G:1182:ASP:OD2	1:G:1193:TYR:OH	2.08	0.55
1:J:485:GLU:O	1:J:489:MET:HG2	2.06	0.55
1:J:1146:TYR:HH	3:L:9:DC:P	2.29	0.55
1:A:417:PHE:HA	1:A:421:ILE:HB	1.88	0.55
1:G:1123:VAL:O	4:G:1301:HOH:O	2.18	0.55
1:G:875:CYS:SG	1:G:876:PHE:N	2.80	0.55
1:J:1040:ILE:HG22	1:J:1042:GLY:H	1.71	0.55
3:L:11:DT:H2'	3:L:12:DA:C8	2.42	0.55
1:G:1026:LYS:O	1:G:1030:ASN:ND2	2.41	0.54
1:J:1124:LEU:HD23	1:J:1208:THR:HG21	1.89	0.54
1:J:1133:PHE:HZ	1:J:1206:ILE:HD13	1.72	0.54
1:J:1180:CYS:O	1:J:1191:ARG:HB3	2.07	0.54
1:A:410:MET:HE2	1:A:434:PRO:HB3	1.88	0.54
1:A:615:GLU:OE1	1:A:650:ARG:NH2	2.36	0.54
1:D:709:SER:HA	1:D:720:ARG:HD3	1.89	0.54
1:J:841:GLY:O	1:J:981:ARG:NH1	2.35	0.54
1:G:1018:VAL:O	1:G:1022:GLY:N	2.38	0.54
2:K:13:DA:H2'	2:K:14:DA:C8	2.43	0.54
1:A:632:ASP:OD1	1:A:664:ARG:NH2	2.35	0.53
1:J:898:ILE:HG22	1:J:899:PRO:HD3	1.91	0.53
1:D:1081:ARG:NH2	1:D:1083:ASP:OD1	2.41	0.53
2:E:12:DG:H2'	2:E:13:DA:C8	2.43	0.53
1:J:1146:TYR:N	1:J:1147:PRO:HD3	2.23	0.53
1:J:537:LEU:HG	1:J:570:LEU:HD21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:875:CYS:SG	1:J:876:PHE:N	2.82	0.53
1:J:1081:ARG:NH2	1:J:1083:ASP:OD2	2.42	0.53
1:G:391:PRO:HB3	1:G:413:VAL:HG21	1.91	0.53
1:J:1222:ARG:NH2	2:K:12:DG:OP1	2.42	0.53
1:J:863:SER:HB3	1:J:866:PRO:HG2	1.91	0.53
1:G:383:ILE:HG12	1:G:523:PRO:HG3	1.90	0.52
1:G:1045:LYS:NZ	4:G:1303:HOH:O	2.28	0.52
1:A:385:ARG:HE	1:A:459:ALA:HA	1.74	0.52
1:A:439:TYR:CZ	1:A:441:PHE:HB2	2.44	0.52
1:A:921:ARG:NH2	4:A:1304:HOH:O	2.43	0.52
1:D:915:ILE:HD11	1:D:956:MET:HG2	1.90	0.52
1:J:1182:ASP:OD1	1:J:1183:GLY:N	2.43	0.52
1:G:498:TRP:CD1	1:G:532:VAL:HG23	2.45	0.52
1:A:1052:LYS:HD3	2:B:9:DG:H5''	1.92	0.51
1:J:793:LEU:HD21	1:J:966:ARG:HH11	1.75	0.51
1:D:545:LYS:HE2	1:D:723:ILE:HD12	1.90	0.51
1:G:929:MET:HE2	1:G:942:TYR:HB3	1.91	0.51
1:J:616:ARG:NH2	1:J:655:LYS:O	2.44	0.51
1:A:705:SER:HB3	1:A:710:GLU:HG2	1.93	0.51
1:G:417:PHE:HA	1:G:421:ILE:HB	1.92	0.51
1:G:841:GLY:O	1:G:981:ARG:HD2	2.11	0.51
1:J:1079:ILE:HA	1:J:1089:LYS:HG2	1.93	0.51
1:A:369:SER:HA	1:D:921:ARG:HH22	1.76	0.51
1:J:595:PRO:HG2	1:J:598:PHE:HB2	1.93	0.51
1:G:922:ARG:NH1	1:G:946:GLN:OE1	2.44	0.51
1:A:692:ASP:H	1:A:781:MET:HE1	1.75	0.51
1:G:446:VAL:HG21	1:G:477:PHE:HZ	1.76	0.51
1:D:458:SER:HB3	1:D:461:MET:HE2	1.94	0.50
1:G:794:HIS:O	1:G:798:GLU:HG2	2.11	0.50
1:A:1000:TYR:HB2	1:A:1049:LEU:HD21	1.93	0.50
1:G:748:ASP:O	1:G:752:ILE:HG12	2.11	0.50
1:G:999:ILE:HD11	1:G:1009:ASN:HB2	1.92	0.50
2:H:12:DG:H2'	2:H:13:DA:C8	2.46	0.50
1:G:667:ARG:NH2	1:G:683:ASN:O	2.44	0.50
1:G:767:GLN:O	1:G:771:ILE:HG12	2.11	0.50
1:J:557:ILE:HG13	1:J:650:ARG:HG3	1.93	0.50
1:D:484:LEU:HD21	1:D:775:ILE:HD11	1.93	0.50
1:D:500:GLU:HB2	1:D:529:ILE:HD11	1.92	0.50
1:G:442:GLU:HG2	1:G:443:ILE:N	2.26	0.50
1:J:1085:CYS:HB2	1:J:1133:PHE:HA	1.93	0.50
1:A:1123:VAL:HG12	1:A:1208:THR:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:969:ALA:HB1	1:G:972:LEU:HB2	1.94	0.50
1:G:627:HIS:HB2	1:G:661:LYS:HD2	1.94	0.49
1:A:375:SER:OG	1:A:630:ASP:OD2	2.28	0.49
1:G:881:ARG:HD2	1:G:971:PRO:HG2	1.95	0.49
1:G:979:LYS:O	1:G:983:ILE:HG12	2.12	0.49
1:A:704:LYS:O	1:A:1082:ARG:NH1	2.45	0.49
1:D:1158:ALA:HB2	1:D:1175:VAL:HG21	1.94	0.49
1:J:439:TYR:CZ	1:J:441:PHE:HB2	2.48	0.49
1:J:1212:LEU:HD22	1:J:1239:LEU:HD21	1.95	0.49
1:J:900:GLU:HG3	1:J:901:LEU:HD13	1.95	0.49
1:J:1047:LEU:HD12	1:J:1057:ALA:HB2	1.94	0.49
3:C:11:DT:H2'	3:C:12:DA:C8	2.48	0.49
1:A:805:ASP:OD2	4:A:1301:HOH:O	2.19	0.49
1:D:1048:LEU:HD22	1:D:1099:ILE:HG21	1.93	0.48
1:D:1079:ILE:HG22	1:D:1089:LYS:HA	1.94	0.48
1:G:1179:ILE:HD12	1:G:1210:TYR:CE2	2.48	0.48
1:G:1182:ASP:CG	1:G:1183:GLY:H	2.19	0.48
1:J:633:ILE:HG12	1:J:689:MET:HB2	1.95	0.48
1:J:702:ARG:HA	1:J:706:TYR:OH	2.13	0.48
1:A:1056:ALA:HB2	1:A:1077:LEU:HD11	1.95	0.48
1:G:549:ASN:O	1:G:553:HIS:HA	2.13	0.48
1:A:926:LYS:HD3	1:A:929:MET:HE2	1.95	0.48
1:D:785:SER:HB3	2:E:5:DG:H5'	1.96	0.48
1:J:601:VAL:HG11	1:J:735:SER:HB3	1.96	0.48
1:A:595:PRO:HB2	1:A:735:SER:HB3	1.95	0.48
1:G:1083:ASP:OD1	1:G:1083:ASP:N	2.43	0.48
1:A:437:LYS:HB2	1:A:452:TYR:CD1	2.49	0.47
1:A:794:HIS:O	1:A:798:GLU:HG2	2.14	0.47
1:A:857:LEU:HD21	1:A:1022:GLY:HA2	1.94	0.47
1:D:547:MET:HE2	1:D:558:ILE:HG21	1.96	0.47
1:A:1194:ALA:HB3	1:A:1197:GLN:HG3	1.95	0.47
1:A:1015:LEU:HD11	1:A:1068:TYR:HD1	1.79	0.47
1:D:658:HIS:HB3	1:D:661:LYS:HG3	1.97	0.47
1:D:1195:PRO:O	1:D:1199:GLN:NE2	2.46	0.47
1:J:1167:ARG:NH2	4:J:1302:HOH:O	2.39	0.47
1:D:434:PRO:HA	1:D:453:LEU:HA	1.96	0.47
1:D:903:ASP:OD1	1:D:903:ASP:N	2.45	0.47
1:G:639:ILE:HG22	1:G:644:LEU:HB2	1.97	0.47
1:G:662:ILE:HG13	1:G:685:THR:HG22	1.96	0.47
1:D:555:ASN:OD1	1:D:555:ASN:N	2.47	0.47
1:A:847:PRO:HB3	1:A:1000:TYR:CD1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:CYS:SG	1:A:876:PHE:N	2.88	0.47
1:D:875:CYS:SG	1:D:876:PHE:N	2.87	0.47
1:J:632:ASP:HA	1:J:664:ARG:HH21	1.80	0.47
1:A:922:ARG:NH1	1:A:946:GLN:OE1	2.48	0.47
1:J:1078:ASP:OD2	1:J:1222:ARG:NH1	2.48	0.47
1:J:1019:PHE:O	1:J:1023:ASN:ND2	2.47	0.47
1:D:385:ARG:O	1:D:456:LYS:HA	2.15	0.47
1:D:600:GLU:OE1	1:D:600:GLU:N	2.47	0.47
1:G:385:ARG:O	1:G:456:LYS:HA	2.15	0.47
1:D:1095:VAL:HG13	1:D:1112:ILE:HD13	1.96	0.46
1:G:646:VAL:O	1:G:650:ARG:HG2	2.15	0.46
1:G:675:GLY:HA2	1:G:678:GLY:HA2	1.97	0.46
1:G:1059:VAL:N	1:G:1071:LYS:O	2.48	0.46
1:D:358:VAL:HG11	1:D:379:MET:HE3	1.97	0.46
1:A:537:LEU:HD11	1:A:570:LEU:HD11	1.98	0.46
1:D:557:ILE:HD12	1:D:619:LEU:HD21	1.96	0.46
1:J:1039:ASP:OD1	1:J:1040:ILE:N	2.45	0.46
1:D:767:GLN:O	1:D:771:ILE:HG12	2.16	0.46
1:J:375:SER:OG	1:J:630:ASP:OD2	2.32	0.46
1:D:390:LEU:HD12	1:D:391:PRO:HD2	1.98	0.46
1:G:436:GLU:HA	1:G:451:GLU:HA	1.97	0.46
1:J:341:PHE:HB3	1:J:501:VAL:HB	1.97	0.46
1:A:796:PHE:HB3	1:A:801:TYR:HB2	1.98	0.46
1:G:929:MET:HE1	1:G:946:GLN:HG2	1.97	0.46
1:G:1123:VAL:HG12	1:G:1208:THR:HG23	1.96	0.46
1:J:460:GLU:OE1	1:J:460:GLU:N	2.45	0.46
1:J:962:PHE:CZ	1:J:964:TYR:HB2	2.50	0.46
1:A:399:ASN:OD1	1:A:400:THR:N	2.46	0.46
1:G:1205:THR:OG1	1:G:1206:ILE:N	2.50	0.45
1:J:775:ILE:HB	1:J:778:ARG:HG2	1.99	0.45
1:A:651:ILE:HG23	1:A:656:ALA:HB3	1.98	0.45
1:A:843:LEU:HD23	1:A:984:LEU:HD23	1.97	0.45
2:B:12:DG:H2'	2:B:13:DA:C8	2.51	0.45
1:D:727:ASN:O	1:D:731:MET:HG2	2.16	0.45
1:G:389:PHE:HB2	1:G:453:LEU:HB3	1.98	0.45
1:D:843:LEU:HD23	1:D:984:LEU:HD23	1.98	0.45
1:J:898:ILE:CG2	1:J:899:PRO:HD3	2.46	0.45
1:A:720:ARG:HH21	1:A:748:ASP:CG	2.25	0.45
3:F:11:DT:H2'	3:F:12:DA:C8	2.51	0.45
1:J:549:ASN:ND2	1:J:554:GLN:O	2.37	0.45
1:J:843:LEU:HD23	1:J:984:LEU:HD23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:GLN:NE2	1:D:941:GLN:OE1	2.44	0.45
1:J:875:CYS:HB2	1:J:912:PRO:HD3	1.98	0.45
1:G:388:TYR:CE1	1:G:437:LYS:HE3	2.52	0.45
1:J:489:MET:HE1	1:J:794:HIS:HA	1.99	0.45
1:G:403:GLU:OE1	1:G:403:GLU:N	2.34	0.44
1:J:1059:VAL:N	1:J:1071:LYS:O	2.49	0.44
1:D:417:PHE:CZ	1:D:455:VAL:HG11	2.53	0.44
1:D:990:MET:HE1	1:D:1032:LEU:HD11	2.00	0.44
1:A:384:GLU:HG3	1:A:456:LYS:HD3	1.99	0.44
1:A:858:LEU:HD13	1:A:1007:MET:HG2	2.00	0.44
1:G:909:GLY:C	1:G:912:PRO:HD2	2.43	0.44
2:K:15:DG:H2"	2:K:16:DG:H5"	2.00	0.44
1:A:634:ILE:HB	1:A:690:ILE:HD13	2.00	0.44
1:D:709:SER:OG	1:D:720:ARG:NH1	2.51	0.44
1:A:935:ASN:HD22	1:A:938:LEU:HD13	1.83	0.43
1:G:395:LYS:O	1:G:403:GLU:HB2	2.18	0.43
1:J:637:HIS:ND1	1:J:752:ILE:HD11	2.33	0.43
1:A:780:LEU:O	1:A:781:MET:HE2	2.18	0.43
1:G:698:LYS:HG3	1:G:706:TYR:CE2	2.53	0.43
1:G:1182:ASP:OD1	1:G:1183:GLY:N	2.33	0.43
1:D:850:GLY:HA2	1:D:1226:PRO:HB3	2.00	0.43
1:D:1148:ASP:OD2	1:D:1148:ASP:N	2.52	0.43
1:J:640:TYR:CD2	1:J:781:MET:HE2	2.54	0.43
1:J:922:ARG:NH1	1:J:946:GLN:OE1	2.52	0.43
1:D:1210:TYR:HE2	1:D:1215:GLN:HE21	1.66	0.43
1:G:977:THR:O	1:G:981:ARG:HD3	2.18	0.43
1:G:935:ASN:HB3	1:G:938:LEU:HD12	2.00	0.43
1:J:708:LEU:O	1:J:712:VAL:HG23	2.18	0.43
1:J:929:MET:HE2	1:J:929:MET:HB3	1.92	0.43
1:A:492:LYS:HE3	1:A:798:GLU:OE1	2.19	0.43
1:D:712:VAL:HG13	1:D:716:LEU:HD12	2.00	0.43
1:A:931:GLN:HB2	1:A:934:LEU:HD22	2.01	0.43
1:G:375:SER:OG	1:G:630:ASP:OD2	2.26	0.43
1:G:437:LYS:HB3	1:G:802:ILE:HG13	2.01	0.43
1:J:634:ILE:HB	1:J:690:ILE:HD13	2.01	0.43
1:D:346:LEU:HD11	1:D:537:LEU:HD22	2.01	0.42
1:D:863:SER:HB2	1:D:866:PRO:HG2	2.01	0.42
1:J:385:ARG:O	1:J:456:LYS:HA	2.19	0.42
1:J:1146:TYR:HD2	1:J:1146:TYR:O	2.02	0.42
1:J:1208:THR:O	1:J:1212:LEU:HG	2.19	0.42
1:A:1124:LEU:HB3	1:A:1208:THR:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:DG:H2''	2:B:16:DG:H5''	2.01	0.42
1:D:633:ILE:HG12	1:D:689:MET:HE2	2.00	0.42
1:G:592:CYS:SG	1:G:729:GLN:HG3	2.59	0.42
1:A:711:LEU:HD13	1:A:711:LEU:HA	1.90	0.42
1:A:711:LEU:HB3	1:A:755:ILE:HD13	2.02	0.42
1:D:425:TYR:O	1:D:462:PRO:HG2	2.19	0.42
1:J:491:ARG:NH2	1:J:527:ASN:OD1	2.51	0.42
1:A:692:ASP:H	1:A:781:MET:CE	2.33	0.42
1:A:958:GLY:HA3	2:B:5:DG:C8	2.54	0.42
1:D:585:VAL:HG22	1:D:618:LEU:HD12	2.02	0.42
1:D:665:LEU:HD12	1:D:665:LEU:HA	1.91	0.42
1:D:1019:PHE:O	1:D:1023:ASN:ND2	2.40	0.42
2:H:7:DT:H2''	2:H:8:DA:C8	2.55	0.42
1:A:878:THR:HB	1:A:902:PRO:HG3	2.01	0.42
1:A:879:VAL:HB	1:A:899:PRO:HB2	2.00	0.42
1:G:395:LYS:CB	1:G:408:ILE:HD11	2.41	0.42
1:G:921:ARG:O	1:G:925:VAL:HG23	2.20	0.42
1:G:996:LEU:HD11	1:G:1021:LEU:HD11	2.02	0.42
1:D:860:ASP:HA	1:D:1005:SER:HA	2.00	0.42
1:D:1098:GLN:HB3	1:D:1108:ILE:HG23	2.02	0.42
1:G:1039:ASP:OD1	1:G:1040:ILE:N	2.52	0.42
1:D:487:PHE:HD1	1:D:523:PRO:HB3	1.84	0.42
1:G:856:ILE:HB	1:G:1044:PHE:HB2	2.01	0.42
1:G:1050:LEU:HD21	1:G:1223:ILE:HA	2.02	0.42
1:J:933:ASP:O	1:J:934:LEU:HB3	2.20	0.42
1:A:437:LYS:HB3	1:A:802:ILE:HG13	2.02	0.41
1:A:722:VAL:HA	1:A:744:HIS:CE1	2.55	0.41
1:A:772:ALA:HA	1:A:791:LEU:HD12	2.02	0.41
1:D:390:LEU:HD22	1:D:446:VAL:HG12	2.02	0.41
1:D:1180:CYS:O	1:D:1191:ARG:NH1	2.53	0.41
1:D:1222:ARG:HH21	2:E:12:DG:P	2.43	0.41
1:G:1084:TRP:HZ3	1:G:1215:GLN:HA	1.85	0.41
1:J:444:PRO:O	1:J:446:VAL:HG23	2.20	0.41
1:J:1052:LYS:HD3	2:K:9:DG:H5''	2.02	0.41
1:D:879:VAL:HG22	1:D:902:PRO:HD3	2.01	0.41
1:G:492:LYS:NZ	1:G:798:GLU:OE1	2.52	0.41
1:A:441:PHE:HB3	1:A:442:GLU:OE1	2.20	0.41
1:D:1095:VAL:O	1:D:1099:ILE:HG12	2.20	0.41
1:D:1179:ILE:HG13	1:D:1210:TYR:CE2	2.56	0.41
1:J:366:TRP:CZ3	1:J:371:GLU:O	2.73	0.41
1:J:988:LYS:HG3	1:J:998:VAL:HG11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:LEU:HB2	1:A:763:PRO:HD3	2.02	0.41
1:G:922:ARG:NH1	1:G:950:LYS:HB2	2.36	0.41
1:J:341:PHE:HB2	1:J:504:PRO:HG3	2.03	0.41
1:J:788:ASN:HD21	1:J:959:CYS:HB2	1.86	0.41
1:A:385:ARG:O	1:A:456:LYS:HA	2.21	0.41
1:D:723:ILE:HD13	1:D:731:MET:HE2	2.03	0.41
1:G:636:GLY:HA3	1:G:639:ILE:HD11	2.01	0.41
1:G:1211:TYR:O	1:G:1216:ILE:HG12	2.20	0.41
1:A:858:LEU:HD11	1:A:1005:SER:HB2	2.02	0.41
1:G:390:LEU:HD12	1:G:391:PRO:HD2	2.02	0.41
1:D:1138:ALA:HA	1:D:1174:THR:HA	2.02	0.41
1:G:341:PHE:HB3	1:G:501:VAL:HB	2.03	0.41
1:G:1163:SER:C	1:G:1165:GLY:H	2.29	0.41
1:J:1078:ASP:N	1:J:1078:ASP:OD1	2.54	0.41
1:D:552:ASN:OD1	1:D:553:HIS:N	2.55	0.40
1:G:365:VAL:HG13	1:G:376:CYS:SG	2.62	0.40
1:G:1044:PHE:HE1	1:G:1059:VAL:HG22	1.86	0.40
1:A:394:MET:HG2	1:A:403:GLU:HG3	2.04	0.40
1:A:708:LEU:O	1:A:712:VAL:HG23	2.21	0.40
1:J:659:TRP:CD2	1:J:670:MET:HG2	2.57	0.40
1:G:511:VAL:O	1:G:666:LYS:HG2	2.21	0.40
1:J:1057:ALA:O	1:J:1073:GLU:N	2.52	0.40
1:J:1241:LEU:HD12	1:J:1241:LEU:HA	1.87	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	A	851/918 (93%)	810 (95%)	41 (5%)	0	100	100
1	D	863/918 (94%)	826 (96%)	37 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	855/918 (93%)	812 (95%)	41 (5%)	2 (0%)	43	71
1	J	853/918 (93%)	804 (94%)	47 (6%)	2 (0%)	43	71
All	All	3422/3672 (93%)	3252 (95%)	166 (5%)	4 (0%)	48	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	406	THR
1	G	1187	THR
1	J	899	PRO
1	J	1146	TYR

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	A	656/824 (80%)	650 (99%)	6 (1%)	70	78
1	D	667/824 (81%)	664 (100%)	3 (0%)	84	84
1	G	647/824 (78%)	644 (100%)	3 (0%)	81	83
1	J	625/824 (76%)	622 (100%)	3 (0%)	81	83
All	All	2595/3296 (79%)	2580 (99%)	15 (1%)	78	81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	LEU
1	A	611	VAL
1	A	711	LEU
1	A	901	LEU
1	A	1067	ASN
1	A	1175	VAL
1	D	499	LEU
1	D	949	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	998	VAL
1	G	410	MET
1	G	901	LEU
1	G	1015	LEU
1	J	635	VAL
1	J	901	LEU
1	J	1241	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	555	ASN
1	A	566	HIS
1	A	1009	ASN
1	A	1011	ASN
1	A	1122	ASN
1	A	1181	GLN
1	D	342	HIS
1	D	627	HIS
1	D	649	GLN
1	D	754	GLN
1	D	770	ASN
1	D	788	ASN
1	D	1201	GLN
1	G	548	GLN
1	G	1122	ASN
1	G	1125	ASN
1	J	509	GLN
1	J	658	HIS
1	J	870	GLN
1	J	1201	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	859/918 (93%)	-0.37	6 (0%) 84 70	42, 93, 164, 222	0
1	D	871/918 (94%)	-0.32	1 (0%) 92 90	42, 103, 167, 224	0
1	G	863/918 (94%)	-0.25	3 (0%) 90 82	49, 111, 184, 248	0
1	J	861/918 (93%)	-0.27	4 (0%) 87 76	45, 110, 181, 233	0
2	B	15/16 (93%)	-0.56	0 100 100	63, 88, 125, 166	0
2	E	16/16 (100%)	-0.28	0 100 100	95, 134, 210, 235	0
2	H	13/16 (81%)	-0.08	0 100 100	101, 174, 270, 272	0
2	K	15/16 (93%)	-0.11	0 100 100	80, 119, 196, 201	0
3	C	13/13 (100%)	-0.59	0 100 100	81, 90, 99, 105	0
3	F	13/13 (100%)	-0.29	0 100 100	94, 123, 224, 228	0
3	I	10/13 (76%)	-0.38	0 100 100	117, 133, 215, 245	0
3	L	13/13 (100%)	-0.37	0 100 100	86, 109, 242, 258	0
All	All	3562/3788 (94%)	-0.30	14 (0%) 88 79	42, 104, 178, 272	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	598	PHE	3.0
1	G	1091	THR	2.5
1	J	1211	TYR	2.4
1	J	1216	ILE	2.4
1	J	1003	THR	2.4
1	G	959	CYS	2.4
1	A	1224	CYS	2.3
1	A	1197	GLN	2.3
1	D	1212	LEU	2.2
1	A	742	LEU	2.2
1	G	1128	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	1245	GLN	2.1
1	A	584	CYS	2.1
1	A	671	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.