Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 06:38 AM EDT

PDB ID	:	3BDN
Title	:	Crystal Structure of the Lambda Repressor
Authors	:	Stayrook, S.E.; Jaru-Ampornpan, P.; Hochschild, A.; Lewis, M.
Deposited on	:	2007-11-15
Resolution	:	3.91 Å(reported)

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

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

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

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

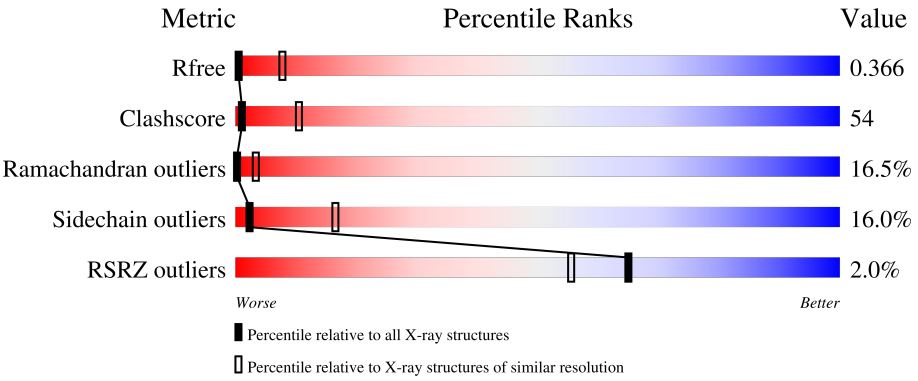
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.91 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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

Mol	Chain	Length	Quality of chain
1	C	20	5% 50% 40% 5%
2	D	20	15% 55% 25% 5%
3	A	236	3% 24% 55% 17%
3	B	236	% 25% 47% 24%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4405 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 DNA (5'-D(*DAP*DAP*DTP*DAP*DCP*DCP*DAP*DCP*DTP*DGP*DGP*DCP*DGP*DGP*DTP*DGP*DAP*DTP*DAP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	19	391	186	72	114	19	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*DTP*DAP*DTP*DAP*DTP*DCP*DAP*DCP*DCP*DGP*DCP*DCP*DAP*DGP*DTP*DGP*DGP*DTP*DAP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	19	388	185	70	114	19	0	0	0

- Molecule 3 is a protein called Lambda Repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	234	1814	1154	298	352	10	0	0	0
3	B	234	Total	C	N	O	S	0	0	0
			1812	1152	298	352	10			

There are 2 discrepancies between the modelled and reference sequences:

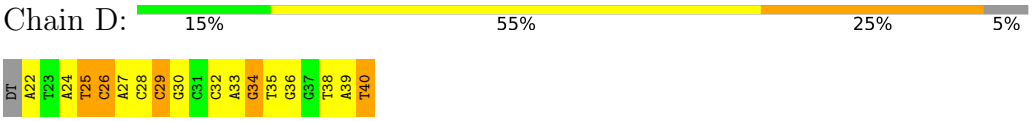
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLY	ASP	engineered mutation	UNP P03034
B	197	GLY	ASP	engineered mutation	UNP P03034

3 Residue-property plots (i)

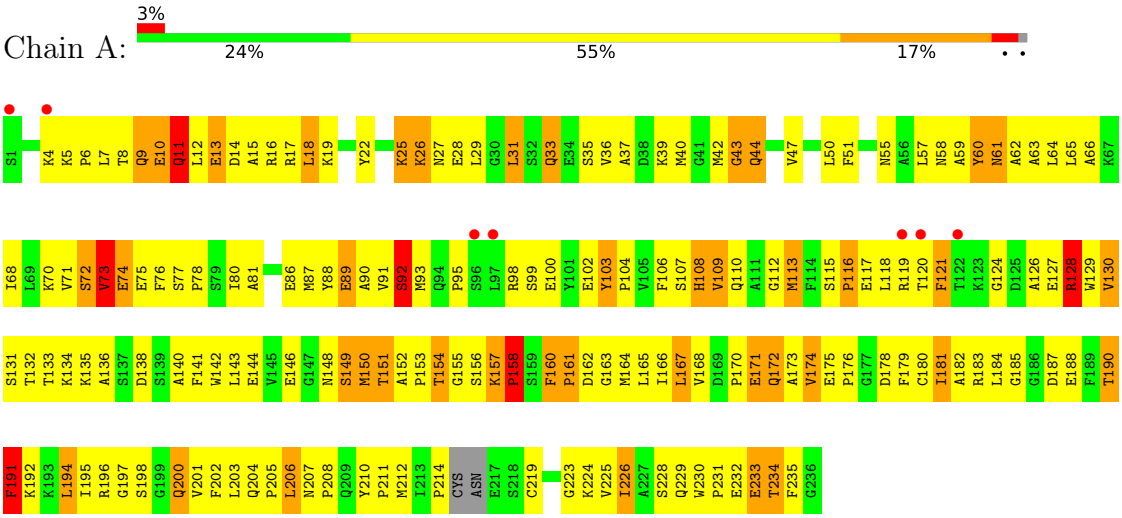
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (5'-D(*DAP*DAP*DTP*DAP*DCP*DCP*DAP*DCP*DTP*DGP*DGP*DCP*DGP*DGP*DTP*DGP*DAP*DTP*DAP*DT)-3')

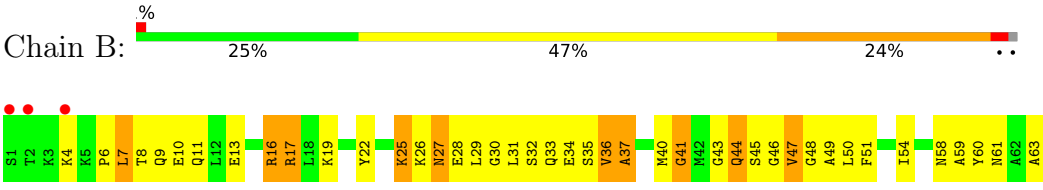
• Molecule 2: DNA (5'-D(*DTP*DAP*DTP*DAP*DTP*DCP*DAP*DCP*DCP*DGP*DCP*DCP*DAP*DGP*DTP*DGP*DGP*DTP*DAP*DT)-3')

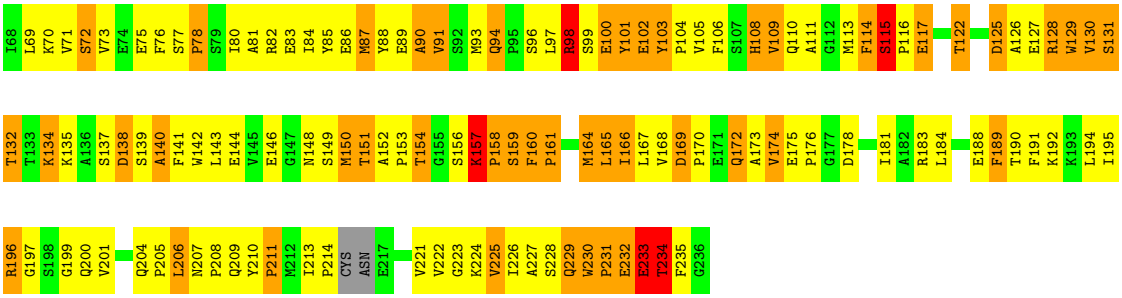


• Molecule 3: Lambda Repressor



• Molecule 3: Lambda Repressor




I68 L69 K70 V71 S72 V73 E74 E75 F76 S77 P78 S79 I80 A81 R82 E83 I84 Y85 E86 M87 Y88 E89 A90 V91 S92 M93 Q94 P95 S96 L97 R98 S99 E100 Y101 E102 Y103 P104 V105 F106 S107 H108 V109 Q110 A111 G112 M113 F114 S115 P116 E117 T122 D125 A126 E127 R128 W129 V130 S131
T132 T133 K134 K135 A136 S137 D138 S139 A140 F141 W142 L143 E144 V145 E146 G147 N148 S149 M150 T151 A152 P153 T154 G155 S156 K157 P158 S159 F160 P161 M164 L165 I166 L167 V168 D169 P170 E171 Q172 A173 V174 E175 P176 G177 D178 I181 A182 R183 L184 E188 F189 T190 F191 K192 K193 L194 I195
R196 G197 S198 G199 Q200 V201 Q204 P205 L206 N207 P208 Q209 Y210 P211 M212 I213 P214 CYS ASN E217 V221 V222 G223 K224 V225 I226 A227 S228 Q229 W230 P231 E232 E233 T234 F235 G236

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	74.43Å 161.10Å 135.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.61 – 3.91 34.60 – 3.91	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.61-3.91) 98.9 (34.60-3.91)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.12 (at 3.87Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.292 , 0.374 0.285 , 0.366	Depositor DCC
R_{free} test set	350 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	150.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 88.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4405	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	C	0.95	0/438	1.88	26/674 (3.9%)
2	D	1.02	1/434 (0.2%)	1.82	15/667 (2.2%)
3	A	1.12	9/1853 (0.5%)	0.95	6/2500 (0.2%)
3	B	1.04	7/1851 (0.4%)	0.89	2/2497 (0.1%)
All	All	1.06	17/4576 (0.4%)	1.18	49/6338 (0.8%)

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
3	A	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	128	ARG	CZ-NH1	23.18	1.63	1.33
3	B	25	LYS	CE-NZ	17.80	1.93	1.49
3	A	25	LYS	CE-NZ	16.20	1.89	1.49
3	A	119	ARG	CZ-NH1	10.27	1.46	1.33
3	B	157	LYS	CE-NZ	8.70	1.70	1.49
2	D	22	DA	P-OP2	8.07	1.62	1.49
3	B	100	GLU	CD-OE2	6.66	1.32	1.25
3	A	100	GLU	CD-OE1	6.56	1.32	1.25
3	A	128	ARG	CD-NE	6.42	1.57	1.46
3	B	13	GLU	CD-OE1	6.40	1.32	1.25
3	B	146	GLU	CD-OE1	6.36	1.32	1.25
3	B	146	GLU	CD-OE2	6.29	1.32	1.25
3	A	92	SER	CB-OG	6.05	1.50	1.42
3	A	100	GLU	CD-OE2	5.53	1.31	1.25
3	B	100	GLU	CD-OE1	5.51	1.31	1.25
3	A	119	ARG	CD-NE	5.47	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	102	GLU	CD-OE1	5.41	1.31	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	119	ARG	NE-CZ-NH2	-12.45	114.08	120.30
3	A	128	ARG	NE-CZ-NH1	12.11	126.36	120.30
2	D	38	DT	O4'-C1'-N1	11.37	115.96	108.00
3	A	128	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	C	5	DC	O4'-C1'-N1	9.23	114.46	108.00
2	D	29	DC	O4'-C1'-N1	9.19	114.44	108.00
2	D	40	DT	O4'-C1'-N1	8.86	114.20	108.00
2	D	27	DA	O4'-C4'-C3'	-8.63	100.82	106.00
1	C	4	DA	O4'-C4'-C3'	-8.55	100.87	106.00
1	C	15	DT	O4'-C1'-N1	8.44	113.91	108.00
2	D	40	DT	C1'-O4'-C4'	-8.17	101.93	110.10
3	A	119	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	C	16	DG	C1'-O4'-C4'	-7.62	102.48	110.10
2	D	38	DT	C1'-O4'-C4'	-7.61	102.49	110.10
1	C	13	DG	O4'-C1'-N9	7.49	113.25	108.00
1	C	13	DG	C1'-O4'-C4'	-6.97	103.13	110.10
2	D	26	DC	O4'-C1'-N1	6.96	112.87	108.00
1	C	9	DT	O4'-C1'-N1	6.92	112.84	108.00
1	C	5	DC	C1'-O4'-C4'	-6.63	103.47	110.10
3	A	119	ARG	NH1-CZ-NH2	6.55	126.60	119.40
2	D	26	DC	C1'-O4'-C4'	-6.51	103.59	110.10
2	D	38	DT	C3'-C2'-C1'	-6.49	94.71	102.50
3	A	128	ARG	CD-NE-CZ	-6.34	114.73	123.60
1	C	15	DT	C1'-O4'-C4'	-6.30	103.80	110.10
1	C	11	DG	C1'-O4'-C4'	-6.27	103.83	110.10
3	B	165	LEU	CA-CB-CG	-6.26	100.89	115.30
2	D	39	DA	P-O3'-C3'	6.02	126.92	119.70
1	C	6	DC	O4'-C1'-N1	5.81	112.07	108.00
1	C	16	DG	O4'-C1'-C2'	-5.80	101.26	105.90
1	C	12	DC	P-O3'-C3'	5.73	126.58	119.70
2	D	25	DT	O4'-C1'-C2'	-5.72	101.32	105.90
1	C	9	DT	C1'-O4'-C4'	-5.70	104.40	110.10
1	C	20	DT	O4'-C4'-C3'	-5.64	102.24	104.50
1	C	9	DT	C5-C4-O4	-5.63	120.96	124.90
1	C	7	DA	O4'-C1'-N9	5.60	111.92	108.00
1	C	9	DT	N3-C4-O4	5.54	123.22	119.90
1	C	18	DT	O4'-C1'-N1	5.51	111.86	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	DA	C1'-O4'-C4'	-5.44	104.66	110.10
1	C	13	DG	O4'-C1'-C2'	-5.44	101.55	105.90
1	C	19	DA	P-O3'-C3'	5.39	126.17	119.70
1	C	9	DT	C3'-C2'-C1'	-5.23	96.22	102.50
3	B	183	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	15	DT	O4'-C1'-C2'	-5.21	101.73	105.90
2	D	26	DC	O4'-C1'-C2'	-5.19	101.75	105.90
1	C	15	DT	N3-C2-O2	-5.13	119.22	122.30
2	D	34	DG	O4'-C1'-N9	5.13	111.59	108.00
1	C	11	DG	O4'-C1'-N9	5.07	111.55	108.00
2	D	28	DC	O4'-C1'-N1	5.07	111.55	108.00
2	D	27	DA	P-O3'-C3'	5.03	125.73	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	157	LYS	Peptide

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	C	391	0	215	20	0
2	D	388	0	215	15	0
3	A	1814	0	1798	207	0
3	B	1812	0	1791	235	0
All	All	4405	0	4019	447	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 54.

All (447) 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)
3:B:157:LYS:CE	3:B:157:LYS:NZ	1.70	1.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:25:LYS:CE	3:A:25:LYS:NZ	1.89	1.33
3:B:25:LYS:CE	3:B:25:LYS:NZ	1.93	1.31
3:B:73:VAL:HG12	3:B:77:SER:O	1.48	1.13
1:C:3:DT:H2"	1:C:4:DA:C8	1.88	1.08
3:B:167:LEU:O	3:B:225:VAL:HA	1.53	1.06
3:B:157:LYS:HB3	3:B:158:PRO:HD3	1.34	1.04
3:A:73:VAL:HA	3:A:76:PHE:CE2	1.93	1.03
3:A:103:TYR:HE2	3:A:136:ALA:HB1	1.24	1.01
3:A:151:THR:HG22	3:A:161:PRO:HA	1.43	1.01
3:A:130:VAL:HA	3:B:132:THR:O	1.62	0.98
3:A:61:ASN:HA	3:A:64:LEU:HD13	1.46	0.96
3:A:151:THR:CG2	3:A:161:PRO:HA	1.96	0.95
3:B:58:ASN:OD1	3:B:60:TYR:HB3	1.66	0.94
1:C:10:DG:H1	2:D:32:DC:H42	0.98	0.94
3:B:103:TYR:HD2	3:B:104:PRO:HD3	1.31	0.93
3:B:208:PRO:C	3:B:210:TYR:H	1.71	0.93
1:C:10:DG:H1	2:D:32:DC:N4	1.68	0.92
3:A:174:VAL:HG22	3:A:224:LYS:HB2	1.53	0.91
3:A:130:VAL:HG13	3:B:132:THR:HB	1.51	0.90
3:A:165:LEU:O	3:A:228:SER:OG	1.91	0.89
3:B:141:PHE:CE2	3:B:168:VAL:HG21	2.09	0.88
3:B:200:GLN:HG2	3:B:201:VAL:H	1.38	0.88
3:B:169:ASP:HB3	3:B:226:ILE:HD11	1.52	0.88
3:A:140:ALA:HB1	3:A:168:VAL:O	1.76	0.86
3:B:33:GLN:HB3	3:B:44:GLN:HG2	1.56	0.85
3:B:181:ILE:CD1	3:B:225:VAL:CG2	2.55	0.85
3:A:103:TYR:CE2	3:A:136:ALA:HB1	2.12	0.85
3:B:61:ASN:HA	3:B:64:LEU:HD22	1.59	0.84
3:A:200:GLN:HG2	3:A:201:VAL:H	1.41	0.83
3:A:190:THR:HB	3:A:192:LYS:NZ	1.95	0.82
3:B:48:GLY:HA2	3:B:51:PHE:HD2	1.44	0.82
3:B:181:ILE:HD11	3:B:225:VAL:CG2	2.10	0.82
3:B:172:GLN:HA	3:B:172:GLN:HE21	1.43	0.81
3:B:181:ILE:HD12	3:B:225:VAL:HG23	1.62	0.80
3:A:78:PRO:HA	3:A:81:ALA:HB3	1.63	0.80
3:B:208:PRO:O	3:B:210:TYR:N	2.15	0.79
3:B:32:SER:O	3:B:35:SER:OG	1.99	0.79
3:B:104:PRO:HA	3:B:128:ARG:HB2	1.64	0.79
3:A:149:SER:HA	3:A:210:TYR:CE2	2.17	0.79
3:A:47:VAL:O	3:A:51:PHE:HE2	1.64	0.79
3:A:39:LYS:O	3:B:117:GLU:HB3	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:103:TYR:CD2	3:B:104:PRO:HD3	2.16	0.78
3:B:157:LYS:CB	3:B:158:PRO:HD3	2.14	0.78
3:B:77:SER:OG	3:B:80:ILE:HG12	1.84	0.77
3:A:138:ASP:HB3	3:A:171:GLU:HG3	1.66	0.77
1:C:17:DA:N6	2:D:25:DT:O4	2.15	0.77
3:A:104:PRO:O	3:A:142:TRP:HB2	1.85	0.76
3:B:181:ILE:CD1	3:B:225:VAL:HG23	2.15	0.76
3:A:37:ALA:HA	3:A:47:VAL:HG21	1.68	0.76
3:A:103:TYR:HB3	3:A:104:PRO:CD	2.15	0.76
3:A:73:VAL:HA	3:A:76:PHE:HE2	1.47	0.76
3:B:208:PRO:C	3:B:210:TYR:N	2.39	0.76
3:B:130:VAL:O	3:B:131:SER:HB2	1.85	0.76
3:B:33:GLN:HB3	3:B:44:GLN:CG	2.15	0.75
3:B:167:LEU:HD23	3:B:226:ILE:HB	1.67	0.75
3:B:98:ARG:HD2	3:B:99:SER:H	1.50	0.74
3:B:165:LEU:O	3:B:228:SER:HA	1.86	0.74
3:B:73:VAL:HA	3:B:76:PHE:CE1	2.22	0.74
3:B:27:ASN:HD22	3:B:27:ASN:H	1.36	0.74
3:A:202:PHE:CD2	3:A:214:PRO:HB3	2.24	0.73
3:B:140:ALA:HA	3:B:169:ASP:HA	1.68	0.73
3:A:73:VAL:O	3:A:76:PHE:N	2.16	0.73
3:A:103:TYR:O	3:A:128:ARG:HG3	1.89	0.73
3:A:10:GLU:C	3:A:12:LEU:H	1.89	0.72
3:A:104:PRO:HA	3:A:128:ARG:HG3	1.70	0.72
3:B:158:PRO:HD2	3:B:206:LEU:HG	1.70	0.72
3:A:36:VAL:HB	3:A:47:VAL:HG11	1.72	0.71
3:B:132:THR:H	3:B:134:LYS:CD	2.03	0.71
3:B:190:THR:OG1	3:B:192:LYS:HE3	1.90	0.71
3:B:104:PRO:HA	3:B:128:ARG:CB	2.20	0.71
3:A:176:PRO:HA	3:A:194:LEU:HB3	1.71	0.71
1:C:10:DG:H2"	1:C:11:DG:C8	2.26	0.70
3:A:72:SER:O	3:A:75:GLU:N	2.15	0.70
3:B:172:GLN:HE21	3:B:172:GLN:CA	2.05	0.70
3:B:200:GLN:HG2	3:B:201:VAL:N	2.06	0.70
3:B:114:PHE:O	3:B:116:PRO:HD2	1.92	0.70
3:A:47:VAL:O	3:A:51:PHE:CE2	2.45	0.70
3:A:149:SER:HA	3:A:210:TYR:HE2	1.55	0.69
3:A:31:LEU:HG	3:A:35:SER:OG	1.92	0.69
3:A:78:PRO:HA	3:A:81:ALA:CB	2.22	0.69
3:A:229:GLN:HB3	3:B:229:GLN:HA	1.75	0.69
3:A:103:TYR:HB3	3:A:104:PRO:HD2	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:8:THR:OG1	3:B:11:GLN:HB2	1.93	0.68
3:A:207:ASN:O	3:A:210:TYR:N	2.20	0.68
3:A:197:GLY:O	3:A:200:GLN:O	2.10	0.68
3:B:169:ASP:CB	3:B:226:ILE:HD11	2.24	0.68
3:A:181:ILE:HA	3:A:191:PHE:HB2	1.76	0.68
3:A:157:LYS:O	3:A:158:PRO:O	2.12	0.67
3:B:17:ARG:HG2	3:B:76:PHE:HA	1.75	0.67
3:B:46:GLY:O	3:B:48:GLY:N	2.27	0.67
3:B:151:THR:H	3:B:207:ASN:HB2	1.60	0.66
3:B:230:TRP:HB3	3:B:231:PRO:CD	2.25	0.66
3:A:58:ASN:OD1	3:A:61:ASN:ND2	2.29	0.66
3:A:187:ASP:HB3	3:A:188:GLU:OE1	1.96	0.65
3:A:14:ASP:O	3:A:17:ARG:HB2	1.97	0.65
3:A:7:LEU:HB2	3:A:12:LEU:HD11	1.78	0.65
3:A:136:ALA:HB1	3:A:140:ALA:HB3	1.79	0.65
3:B:172:GLN:HA	3:B:172:GLN:NE2	2.12	0.65
3:B:157:LYS:HB3	3:B:158:PRO:CD	2.22	0.65
3:B:181:ILE:HD11	3:B:225:VAL:HG22	1.79	0.65
3:A:15:ALA:O	3:A:18:LEU:HB3	1.97	0.64
3:B:224:LYS:O	3:B:226:ILE:HG13	1.97	0.64
3:A:10:GLU:O	3:A:12:LEU:N	2.30	0.64
3:B:131:SER:H	3:B:134:LYS:HE2	1.62	0.64
3:A:26:LYS:HD2	3:A:27:ASN:ND2	2.13	0.64
1:C:16:DG:O6	2:D:26:DC:N4	2.31	0.63
3:B:184:LEU:HD11	3:B:213:ILE:HD13	1.79	0.63
3:B:94:GLN:HE22	3:B:96:SER:HB3	1.64	0.63
1:C:2:DA:N1	2:D:40:DT:O4	2.32	0.62
3:A:31:LEU:HD11	3:A:36:VAL:HG22	1.81	0.62
3:A:204:GLN:HA	3:A:212:MET:HG2	1.82	0.62
3:B:88:TYR:O	3:B:91:VAL:N	2.32	0.62
3:A:205:PRO:HD2	3:A:212:MET:HG2	1.82	0.62
3:A:50:LEU:HA	3:A:55:ASN:HB2	1.81	0.62
3:A:150:MET:SD	3:A:206:LEU:HB2	2.40	0.62
3:A:112:GLY:HA3	3:A:118:LEU:HG	1.82	0.61
3:B:108:HIS:CE1	3:B:144:GLU:HB2	2.35	0.61
3:A:8:THR:O	3:A:12:LEU:HG	2.00	0.61
3:B:130:VAL:HG23	3:B:134:LYS:HE3	1.82	0.61
3:A:150:MET:HG2	3:A:160:PHE:HD1	1.65	0.61
3:B:130:VAL:O	3:B:131:SER:CB	2.49	0.61
3:B:172:GLN:HE21	3:B:173:ALA:H	1.48	0.61
3:A:175:GLU:HB2	3:A:176:PRO:HD2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:167:LEU:HD13	3:A:168:VAL:N	2.16	0.61
3:A:202:PHE:HD2	3:A:214:PRO:HB3	1.65	0.61
3:A:234:THR:O	3:A:234:THR:HG22	1.99	0.61
3:B:150:MET:CE	3:B:192:LYS:HA	2.30	0.61
3:A:10:GLU:C	3:A:12:LEU:N	2.54	0.60
3:A:132:THR:OG1	3:A:133:THR:N	2.34	0.60
3:A:170:PRO:HG3	3:A:223:GLY:HA3	1.83	0.60
3:A:110:GLN:HG2	3:A:112:GLY:H	1.66	0.60
3:B:37:ALA:HB1	3:B:43:GLY:C	2.22	0.60
3:A:168:VAL:HA	3:A:224:LYS:O	2.01	0.60
3:B:93:MET:O	3:B:94:GLN:HB3	2.02	0.60
3:A:171:GLU:O	3:A:172:GLN:HB2	2.00	0.60
3:A:233:GLU:C	3:A:235:PHE:H	2.05	0.60
3:A:183:ARG:CB	3:A:188:GLU:O	2.49	0.60
3:A:146:GLU:HG3	3:A:162:ASP:OD1	2.02	0.60
3:A:200:GLN:HG2	3:A:201:VAL:N	2.16	0.60
3:B:27:ASN:HD22	3:B:27:ASN:N	1.98	0.60
3:A:37:ALA:HA	3:A:47:VAL:CG2	2.32	0.60
3:A:226:ILE:O	3:B:235:PHE:CE1	2.55	0.60
3:B:181:ILE:HD12	3:B:225:VAL:CG2	2.26	0.60
3:A:151:THR:HG23	3:A:161:PRO:HA	1.84	0.59
3:B:105:VAL:O	3:B:143:LEU:HD23	2.02	0.59
3:B:128:ARG:HG3	3:B:128:ARG:O	2.01	0.59
3:A:74:GLU:N	3:A:74:GLU:OE1	2.36	0.59
3:A:103:TYR:HB3	3:A:141:PHE:HA	1.85	0.59
3:A:190:THR:HB	3:A:192:LYS:HZ1	1.67	0.59
1:C:16:DG:C6	1:C:17:DA:C6	2.91	0.59
3:B:10:GLU:HB2	3:B:125:ASP:HB2	1.84	0.58
3:A:229:GLN:HB2	3:B:228:SER:O	2.04	0.58
3:B:141:PHE:CZ	3:B:168:VAL:HG21	2.39	0.58
3:B:87:MET:O	3:B:90:ALA:HB3	2.04	0.58
3:B:73:VAL:O	3:B:77:SER:N	2.33	0.58
3:A:103:TYR:CB	3:A:141:PHE:HA	2.33	0.58
3:A:142:TRP:CD2	3:A:167:LEU:HD23	2.39	0.58
3:A:228:SER:O	3:B:229:GLN:O	2.21	0.58
3:A:64:LEU:O	3:A:68:ILE:HD13	2.05	0.57
3:A:181:ILE:HD13	3:A:182:ALA:H	1.69	0.57
3:A:104:PRO:HA	3:A:128:ARG:CG	2.33	0.57
3:B:48:GLY:HA2	3:B:51:PHE:CD2	2.33	0.56
3:B:72:SER:OG	3:B:73:VAL:N	2.37	0.56
3:B:106:PHE:CZ	3:B:122:THR:HB	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:111:ALA:C	3:B:113:MET:H	2.08	0.56
3:B:152:ALA:O	3:B:154:THR:N	2.38	0.56
3:A:103:TYR:HE2	3:A:136:ALA:CB	2.10	0.56
3:B:88:TYR:O	3:B:89:GLU:C	2.43	0.56
3:B:106:PHE:HZ	3:B:122:THR:HB	1.70	0.56
3:A:229:GLN:OE1	3:B:229:GLN:NE2	2.38	0.56
3:B:78:PRO:O	3:B:81:ALA:HB3	2.05	0.56
1:C:9:DT:H2"	1:C:10:DG:N7	2.21	0.56
3:B:143:LEU:O	3:B:165:LEU:HD23	2.06	0.56
3:B:229:GLN:O	3:B:230:TRP:HB2	2.06	0.56
3:A:203:LEU:O	3:A:212:MET:HG2	2.06	0.56
3:B:164:MET:HG2	3:B:165:LEU:H	1.72	0.55
2:D:35:DT:H2"	2:D:36:DG:OP2	2.07	0.55
3:A:113:MET:O	3:A:116:PRO:HD2	2.07	0.55
3:A:183:ARG:HB3	3:A:188:GLU:O	2.05	0.55
3:B:113:MET:CE	3:B:222:VAL:HG22	2.37	0.55
3:B:125:ASP:CG	3:B:126:ALA:H	2.09	0.55
3:B:148:ASN:O	3:B:207:ASN:ND2	2.39	0.55
3:B:197:GLY:C	3:B:199:GLY:N	2.57	0.55
3:A:37:ALA:HB2	3:A:44:GLN:HG2	1.88	0.54
3:A:191:PHE:O	3:A:192:LYS:HD3	2.07	0.54
3:A:196:ARG:NH2	3:A:198:SER:HA	2.21	0.54
1:C:2:DA:C6	2:D:40:DT:O4	2.60	0.54
3:B:26:LYS:O	3:B:30:GLY:N	2.40	0.54
3:B:141:PHE:O	3:B:167:LEU:HD12	2.07	0.54
3:B:125:ASP:CG	3:B:126:ALA:N	2.59	0.54
3:B:230:TRP:CE3	3:B:231:PRO:HD3	2.42	0.54
3:B:150:MET:HB3	3:B:206:LEU:H	1.73	0.53
3:A:7:LEU:HA	3:A:12:LEU:HD21	1.89	0.53
3:B:101:TYR:CE1	3:B:137:SER:HB3	2.43	0.53
3:A:68:ILE:N	3:A:68:ILE:HD12	2.23	0.53
3:A:87:MET:O	3:A:90:ALA:HB3	2.08	0.53
3:B:138:ASP:OD1	3:B:138:ASP:N	2.41	0.53
3:B:44:GLN:O	3:B:47:VAL:HG23	2.09	0.53
3:B:189:PHE:CD1	3:B:190:THR:HA	2.44	0.53
3:B:66:ALA:HB1	3:B:71:VAL:O	2.08	0.53
3:B:150:MET:HB3	3:B:206:LEU:N	2.23	0.53
3:B:150:MET:CB	3:B:206:LEU:H	2.21	0.53
3:B:172:GLN:NE2	3:B:173:ALA:H	2.07	0.53
3:A:13:GLU:O	3:A:17:ARG:HG3	2.08	0.53
3:A:37:ALA:CA	3:A:47:VAL:HG21	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:VAL:HA	3:A:76:PHE:CD2	2.40	0.53
3:A:184:LEU:HD23	3:A:185:GLY:N	2.24	0.53
3:A:183:ARG:HB2	3:A:188:GLU:O	2.09	0.52
3:B:134:LYS:NZ	3:B:134:LYS:HB3	2.24	0.52
3:A:133:THR:HB	3:B:129:TRP:CZ2	2.45	0.52
3:A:194:LEU:HD13	3:A:202:PHE:O	2.09	0.52
3:B:176:PRO:HB3	3:B:196:ARG:HG2	1.90	0.52
3:B:152:ALA:HB1	3:B:156:SER:HB3	1.91	0.52
3:B:170:PRO:HA	3:B:223:GLY:HA3	1.91	0.52
1:C:13:DG:H2"	1:C:14:DG:H8	1.75	0.52
3:B:47:VAL:HG12	3:B:51:PHE:HE2	1.74	0.52
3:B:233:GLU:C	3:B:235:PHE:H	2.12	0.52
3:A:202:PHE:HD2	3:A:214:PRO:CB	2.22	0.52
3:B:34:GLU:O	3:B:37:ALA:HB3	2.10	0.52
1:C:16:DG:H2"	1:C:17:DA:H8	1.74	0.52
3:A:148:ASN:O	3:A:150:MET:N	2.43	0.52
3:B:159:SER:O	3:B:160:PHE:HD1	1.92	0.52
3:A:15:ALA:HB1	3:A:51:PHE:HA	1.92	0.51
3:A:106:PHE:CE1	3:A:108:HIS:O	2.63	0.51
3:A:136:ALA:CB	3:A:140:ALA:HB3	2.39	0.51
3:B:37:ALA:CB	3:B:43:GLY:C	2.78	0.51
3:A:126:ALA:HB3	3:A:128:ARG:HH11	1.74	0.51
3:B:174:VAL:HG21	3:B:221:VAL:HG11	1.91	0.51
3:B:230:TRP:HE3	3:B:231:PRO:HD3	1.75	0.51
3:A:86:GLU:HA	3:A:89:GLU:OE2	2.10	0.51
3:B:159:SER:O	3:B:160:PHE:CD1	2.64	0.51
3:A:19:LYS:O	3:A:22:TYR:HB3	2.11	0.51
3:A:103:TYR:CB	3:A:104:PRO:CD	2.87	0.51
3:B:153:PRO:HD2	3:B:156:SER:CB	2.41	0.51
3:B:150:MET:HE3	3:B:192:LYS:HA	1.93	0.51
3:A:165:LEU:C	3:A:166:ILE:HG23	2.31	0.51
3:A:205:PRO:HG2	3:A:211:PRO:O	2.11	0.51
3:B:196:ARG:HA	3:B:200:GLN:O	2.11	0.51
3:B:221:VAL:HG22	3:B:222:VAL:H	1.76	0.51
1:C:13:DG:C2	1:C:14:DG:H1'	2.46	0.51
3:A:146:GLU:HA	3:A:162:ASP:OD1	2.11	0.51
3:A:128:ARG:O	3:A:128:ARG:HG2	2.11	0.50
3:B:28:GLU:HG3	3:B:29:LEU:HG	1.92	0.50
3:B:114:PHE:CG	3:B:115:SER:N	2.79	0.50
3:A:88:TYR:O	3:A:91:VAL:HG12	2.12	0.50
3:B:132:THR:H	3:B:134:LYS:HD2	1.73	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:27:ASN:H	3:B:27:ASN:ND2	2.06	0.50
3:A:18:LEU:HD13	3:A:76:PHE:CD1	2.47	0.50
3:A:40:MET:CE	3:A:65:LEU:HD21	2.41	0.50
3:A:131:SER:H	3:B:132:THR:C	2.15	0.50
3:A:133:THR:HG23	3:A:133:THR:O	2.12	0.50
1:C:12:DC:H2"	1:C:13:DG:H8	1.75	0.50
3:B:104:PRO:HD2	3:B:141:PHE:HB3	1.94	0.50
3:A:126:ALA:O	3:A:127:GLU:HB2	2.12	0.50
3:B:96:SER:C	3:B:98:ARG:H	2.14	0.50
2:D:30:DG:H8	2:D:30:DG:OP2	1.95	0.49
3:B:19:LYS:HG3	3:B:51:PHE:HB3	1.93	0.49
3:B:175:GLU:O	3:B:178:ASP:HB2	2.12	0.49
3:A:130:VAL:CA	3:B:132:THR:O	2.49	0.49
3:A:200:GLN:NE2	3:A:202:PHE:CE2	2.80	0.49
3:A:166:ILE:HG22	3:A:228:SER:OG	2.11	0.49
3:A:88:TYR:O	3:A:92:SER:N	2.45	0.49
3:A:98:ARG:NE	3:B:100:GLU:OE2	2.41	0.49
3:A:149:SER:CA	3:A:210:TYR:HE2	2.24	0.49
2:D:29:DC:H2"	2:D:30:DG:C8	2.47	0.49
3:B:32:SER:O	3:B:36:VAL:HG23	2.12	0.49
3:B:137:SER:O	3:B:139:SER:N	2.46	0.49
3:A:184:LEU:HD23	3:A:185:GLY:H	1.77	0.49
3:A:134:LYS:HD3	3:A:135:LYS:O	2.11	0.49
3:B:17:ARG:CZ	3:B:17:ARG:HB2	2.43	0.49
1:C:16:DG:H2"	1:C:17:DA:C8	2.48	0.49
3:B:7:LEU:CD2	3:B:11:GLN:HB3	2.43	0.49
3:B:151:THR:O	3:B:152:ALA:C	2.51	0.49
3:A:129:TRP:CD1	3:A:232:GLU:OE2	2.66	0.48
3:B:29:LEU:HB2	3:B:31:LEU:HD11	1.95	0.48
2:D:40:DT:OP2	2:D:40:DT:H3'	2.14	0.48
3:A:25:LYS:NZ	3:A:25:LYS:CD	2.72	0.48
1:C:11:DG:H4'	1:C:12:DC:OP1	2.12	0.48
2:D:32:DC:H2"	2:D:33:DA:N7	2.29	0.48
3:B:166:ILE:HG21	3:B:191:PHE:CZ	2.48	0.48
3:A:152:ALA:HB1	3:A:156:SER:HB3	1.96	0.48
3:A:170:PRO:HG3	3:A:223:GLY:CA	2.41	0.48
3:A:204:GLN:HA	3:A:212:MET:CG	2.43	0.48
3:B:150:MET:HB2	3:B:206:LEU:HB2	1.96	0.48
1:C:19:DA:H2"	1:C:20:DT:OP2	2.14	0.48
3:A:172:GLN:O	3:A:174:VAL:HG23	2.14	0.48
3:B:106:PHE:HE1	3:B:122:THR:HG1	1.55	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:11:GLN:O	3:A:12:LEU:HD23	2.14	0.48
3:B:234:THR:C	3:B:235:PHE:CG	2.87	0.48
3:B:159:SER:C	3:B:160:PHE:CD1	2.87	0.47
3:A:73:VAL:O	3:A:76:PHE:CD2	2.67	0.47
3:A:130:VAL:HG13	3:B:132:THR:CB	2.31	0.47
3:A:229:GLN:HE22	3:B:132:THR:CB	2.27	0.47
3:B:148:ASN:O	3:B:210:TYR:HE2	1.97	0.47
3:A:10:GLU:HA	3:A:13:GLU:CD	2.35	0.47
3:A:121:PHE:CZ	3:A:124:GLY:HA2	2.50	0.47
2:D:35:DT:P	3:A:42:MET:HB2	2.54	0.47
3:A:235:PHE:CZ	3:B:227:ALA:HA	2.49	0.47
3:B:44:GLN:O	3:B:46:GLY:N	2.48	0.47
3:A:9:GLN:HE22	3:A:13:GLU:HG2	1.80	0.47
3:A:113:MET:HG3	3:A:115:SER:H	1.79	0.47
3:A:157:LYS:C	3:A:158:PRO:O	2.53	0.47
3:A:180:CYS:O	3:A:191:PHE:HD2	1.96	0.47
3:B:78:PRO:O	3:B:81:ALA:N	2.48	0.47
3:B:210:TYR:HB3	3:B:211:PRO:HD2	1.96	0.47
3:A:230:TRP:HE3	3:A:231:PRO:HD3	1.80	0.47
3:B:115:SER:HB2	3:B:116:PRO:HD3	1.97	0.47
3:B:153:PRO:HD2	3:B:156:SER:HB2	1.97	0.47
3:B:157:LYS:NZ	3:B:157:LYS:CD	2.68	0.47
1:C:13:DG:H2"	1:C:14:DG:C8	2.50	0.47
3:A:19:LYS:HA	3:A:22:TYR:HB3	1.97	0.47
3:B:232:GLU:C	3:B:234:THR:N	2.68	0.47
3:A:115:SER:OG	3:A:116:PRO:HD3	2.15	0.47
3:B:113:MET:HE1	3:B:170:PRO:HB3	1.97	0.47
3:A:33:GLN:C	3:A:35:SER:N	2.67	0.46
3:B:16:ARG:O	3:B:19:LYS:N	2.48	0.46
3:A:143:LEU:HD23	3:A:144:GLU:N	2.30	0.46
3:B:37:ALA:HB1	3:B:43:GLY:CA	2.46	0.46
3:B:73:VAL:HA	3:B:76:PHE:HE1	1.75	0.46
3:A:229:GLN:HB3	3:B:229:GLN:HE21	1.80	0.46
3:B:33:GLN:HB3	3:B:44:GLN:HG3	1.97	0.46
3:B:150:MET:CB	3:B:206:LEU:N	2.78	0.46
3:B:157:LYS:CB	3:B:158:PRO:CD	2.86	0.46
3:A:153:PRO:O	3:A:155:GLY:N	2.49	0.46
3:B:49:ALA:O	3:B:54:ILE:N	2.43	0.46
3:B:50:LEU:O	3:B:51:PHE:C	2.52	0.46
3:A:73:VAL:C	3:A:75:GLU:N	2.68	0.46
3:A:164:MET:HG2	3:A:230:TRP:CE3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:49:ALA:HA	3:B:54:ILE:HD12	1.98	0.46
3:B:201:VAL:O	3:B:201:VAL:HG13	2.15	0.46
3:A:74:GLU:HB3	3:A:81:ALA:CB	2.46	0.46
3:B:132:THR:H	3:B:134:LYS:HD3	1.78	0.46
3:A:149:SER:HA	3:A:210:TYR:CD2	2.50	0.46
3:A:229:GLN:HE22	3:B:132:THR:HB	1.81	0.46
3:B:97:LEU:C	3:B:98:ARG:HG3	2.35	0.46
3:A:150:MET:O	3:A:151:THR:C	2.55	0.45
3:B:113:MET:HE2	3:B:222:VAL:HG22	1.96	0.45
3:B:172:GLN:CA	3:B:172:GLN:NE2	2.76	0.45
3:B:140:ALA:O	3:B:141:PHE:HD1	1.99	0.45
3:B:58:ASN:O	3:B:61:ASN:N	2.49	0.45
3:B:140:ALA:HA	3:B:170:PRO:HD3	1.97	0.45
3:B:204:GLN:HA	3:B:205:PRO:HD3	1.80	0.45
3:B:66:ALA:HB1	3:B:72:SER:O	2.15	0.45
3:B:98:ARG:CD	3:B:99:SER:H	2.22	0.45
3:B:159:SER:OG	3:B:160:PHE:N	2.47	0.45
3:B:231:PRO:O	3:B:232:GLU:HB2	2.16	0.45
3:A:130:VAL:HG22	3:B:132:THR:O	2.17	0.45
3:B:210:TYR:HB3	3:B:211:PRO:CD	2.47	0.45
3:A:59:ALA:O	3:A:62:ALA:HB3	2.16	0.45
3:A:230:TRP:HE3	3:A:231:PRO:CD	2.29	0.45
1:C:13:DG:N2	1:C:14:DG:H1'	2.32	0.45
3:B:61:ASN:O	3:B:64:LEU:HB2	2.16	0.45
3:A:126:ALA:HB3	3:A:128:ARG:HD2	1.99	0.45
3:A:181:ILE:HD13	3:A:182:ALA:N	2.31	0.45
3:B:98:ARG:HH21	3:B:101:TYR:H	1.64	0.45
3:A:161:PRO:HB2	3:A:162:ASP:H	1.52	0.45
3:B:17:ARG:HG2	3:B:75:GLU:O	2.16	0.45
3:A:157:LYS:CB	3:A:158:PRO:HD2	2.48	0.44
3:A:190:THR:HB	3:A:192:LYS:CE	2.48	0.44
3:B:82:ARG:HB2	3:B:102:GLU:HG3	1.99	0.44
3:B:167:LEU:HB3	3:B:227:ALA:H	1.82	0.44
3:B:188:GLU:OE2	3:B:188:GLU:N	2.49	0.44
3:A:29:LEU:O	3:A:29:LEU:HD23	2.17	0.44
3:B:36:VAL:O	3:B:37:ALA:C	2.55	0.44
3:B:40:MET:HG3	3:B:41:GLY:H	1.82	0.44
3:B:233:GLU:C	3:B:235:PHE:N	2.70	0.44
3:B:109:VAL:HG22	3:B:110:GLN:O	2.17	0.44
1:C:3:DT:O3'	1:C:4:DA:O4'	2.35	0.44
3:A:148:ASN:C	3:A:150:MET:H	2.20	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:22:TYR:CZ	3:B:26:LYS:HD3	2.52	0.44
3:A:205:PRO:HD2	3:A:212:MET:CG	2.47	0.44
3:A:18:LEU:O	3:A:19:LYS:C	2.55	0.44
3:A:133:THR:HB	3:B:129:TRP:HZ2	1.83	0.44
3:B:26:LYS:HG3	3:B:27:ASN:HD22	1.83	0.44
3:B:114:PHE:O	3:B:116:PRO:CD	2.64	0.44
3:B:150:MET:SD	3:B:150:MET:N	2.91	0.44
3:A:89:GLU:HA	3:A:92:SER:HB3	1.99	0.43
3:B:113:MET:HE3	3:B:222:VAL:HG22	1.99	0.43
3:B:169:ASP:HA	3:B:170:PRO:HD3	1.77	0.43
3:A:106:PHE:CZ	3:A:108:HIS:O	2.71	0.43
3:A:73:VAL:O	3:A:75:GLU:N	2.51	0.43
3:B:158:PRO:CD	3:B:206:LEU:HG	2.44	0.43
3:B:234:THR:HB	3:B:235:PHE:CE1	2.53	0.43
3:A:234:THR:O	3:A:234:THR:CG2	2.65	0.43
3:A:190:THR:HB	3:A:192:LYS:HZ3	1.75	0.43
3:B:80:ILE:O	3:B:83:GLU:HB3	2.19	0.43
3:B:191:PHE:C	3:B:192:LYS:HG2	2.38	0.43
3:B:34:GLU:HA	3:B:44:GLN:HB2	2.01	0.43
3:A:16:ARG:O	3:A:17:ARG:C	2.56	0.43
3:A:33:GLN:C	3:A:35:SER:H	2.21	0.43
3:A:165:LEU:C	3:A:166:ILE:CG2	2.87	0.43
3:B:114:PHE:HD2	3:B:116:PRO:O	2.02	0.43
3:B:137:SER:O	3:B:138:ASP:C	2.56	0.43
3:B:86:GLU:O	3:B:88:TYR:N	2.52	0.43
3:B:172:GLN:HE21	3:B:173:ALA:N	2.13	0.43
3:A:233:GLU:OE2	3:A:234:THR:N	2.52	0.42
2:D:34:DG:H3'	3:A:42:MET:CE	2.49	0.42
2:D:35:DT:P	3:A:43:GLY:H	2.42	0.42
3:A:164:MET:HG2	3:A:230:TRP:CD2	2.53	0.42
3:B:139:SER:HB2	3:B:170:PRO:HG2	2.02	0.42
3:B:205:PRO:O	3:B:207:ASN:N	2.42	0.42
3:B:207:ASN:O	3:B:210:TYR:HB2	2.19	0.42
3:A:5:LYS:HA	3:A:6:PRO:HD2	1.95	0.42
3:A:121:PHE:CE1	3:A:124:GLY:HA2	2.55	0.42
3:A:162:ASP:O	3:A:164:MET:N	2.52	0.42
2:D:24:DA:H2"	2:D:25:DT:H5'	2.01	0.42
3:B:97:LEU:HG	3:B:101:TYR:CE2	2.54	0.42
3:B:151:THR:HG23	3:B:161:PRO:HA	2.02	0.42
3:B:233:GLU:CD	3:B:233:GLU:H	2.23	0.42
3:A:152:ALA:HB1	3:A:153:PRO:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:143:LEU:HD23	3:B:143:LEU:HA	1.75	0.42
3:A:151:THR:HG22	3:A:161:PRO:CA	2.31	0.42
3:A:167:LEU:O	3:A:225:VAL:HA	2.20	0.42
3:B:221:VAL:HG22	3:B:222:VAL:N	2.35	0.42
3:A:60:TYR:O	3:A:63:ALA:N	2.51	0.42
3:A:77:SER:OG	3:A:80:ILE:HG13	2.20	0.42
3:A:192:LYS:HB2	3:A:203:LEU:HB3	2.02	0.42
3:B:207:ASN:HA	3:B:208:PRO:HD2	1.88	0.42
3:B:138:ASP:HB2	3:B:139:SER:H	1.48	0.41
3:B:60:TYR:O	3:B:63:ALA:HB3	2.20	0.41
3:B:142:TRP:CZ3	3:B:167:LEU:HB2	2.55	0.41
3:A:157:LYS:HB3	3:A:158:PRO:HD2	2.01	0.41
3:B:47:VAL:O	3:B:51:PHE:CD2	2.73	0.41
3:B:205:PRO:C	3:B:207:ASN:H	2.24	0.41
3:A:4:LYS:HB3	3:A:5:LYS:H	1.52	0.41
3:A:61:ASN:ND2	3:A:61:ASN:N	2.69	0.41
3:A:66:ALA:O	3:A:70:LYS:N	2.53	0.41
3:B:70:LYS:HA	3:B:70:LYS:HD2	1.94	0.41
3:B:80:ILE:O	3:B:81:ALA:C	2.57	0.41
3:A:50:LEU:HD21	3:A:57:LEU:HG	2.03	0.41
3:B:197:GLY:O	3:B:199:GLY:N	2.54	0.41
3:A:103:TYR:O	3:A:142:TRP:HD1	2.03	0.41
3:A:160:PHE:HA	3:A:161:PRO:HD3	1.64	0.41
3:B:64:LEU:O	3:B:67:LYS:HB2	2.20	0.41
3:B:201:VAL:HG13	3:B:214:PRO:O	2.21	0.41
3:B:85:TYR:O	3:B:86:GLU:C	2.58	0.41
3:B:88:TYR:O	3:B:90:ALA:N	2.54	0.41
3:A:179:PHE:O	3:A:225:VAL:HB	2.20	0.40
3:A:63:ALA:HB1	3:B:87:MET:HA	2.03	0.40
3:A:136:ALA:C	3:A:138:ASP:H	2.25	0.40
3:A:194:LEU:HD22	3:A:203:LEU:HG	2.02	0.40
3:B:37:ALA:HB2	3:B:44:GLN:N	2.37	0.40
3:B:230:TRP:HB3	3:B:231:PRO:HD3	2.02	0.40
3:A:107:SER:O	3:A:109:VAL:HG22	2.22	0.40
3:A:229:GLN:CB	3:B:229:GLN:HA	2.49	0.40
3:B:114:PHE:CD2	3:B:116:PRO:O	2.75	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	230/236 (98%)	136 (59%)	61 (26%)	33 (14%)	0 4
3	B	230/236 (98%)	128 (56%)	59 (26%)	43 (19%)	0 2
All	All	460/472 (98%)	264 (57%)	120 (26%)	76 (16%)	0 3

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	9	GLN
3	A	11	GLN
3	A	73	VAL
3	A	103	TYR
3	A	116	PRO
3	A	120	THR
3	A	154	THR
3	A	158	PRO
3	A	161	PRO
3	A	234	THR
3	B	6	PRO
3	B	45	SER
3	B	47	VAL
3	B	91	VAL
3	B	94	GLN
3	B	114	PHE
3	B	115	SER
3	B	131	SER
3	B	149	SER
3	B	157	LYS
3	B	209	GLN
3	B	225	VAL
3	B	231	PRO
3	A	43	GLY
3	A	60	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	72	SER
3	A	74	GLU
3	A	93	MET
3	A	109	VAL
3	A	121	PHE
3	A	130	VAL
3	A	149	SER
3	A	191	PHE
3	B	41	GLY
3	B	108	HIS
3	B	109	VAL
3	B	128	ARG
3	B	164	MET
3	B	169	ASP
3	B	206	LEU
3	B	232	GLU
3	B	233	GLU
3	A	151	THR
3	A	163	GLY
3	A	171	GLU
3	A	172	GLN
3	A	173	ALA
3	B	7	LEU
3	B	37	ALA
3	B	72	SER
3	B	78	PRO
3	B	158	PRO
3	B	160	PHE
3	B	211	PRO
3	A	95	PRO
3	A	174	VAL
3	A	208	PRO
3	B	59	ALA
3	B	87	MET
3	B	98	ARG
3	B	102	GLU
3	B	127	GLU
3	B	140	ALA
3	B	230	TRP
3	A	18	LEU
3	A	71	VAL
3	A	99	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	113	MET
3	A	160	PHE
3	B	90	ALA
3	B	154	THR
3	B	159	SER
3	B	234	THR
3	B	84	ILE
3	B	36	VAL
3	B	161	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	197/199 (99%)	167 (85%)	30 (15%)	3 17
3	B	196/199 (98%)	163 (83%)	33 (17%)	2 15
All	All	393/398 (99%)	330 (84%)	63 (16%)	2 16

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	GLU
3	A	11	GLN
3	A	13	GLU
3	A	26	LYS
3	A	28	GLU
3	A	31	LEU
3	A	33	GLN
3	A	44	GLN
3	A	61	ASN
3	A	73	VAL
3	A	89	GLU
3	A	92	SER
3	A	108	HIS
3	A	117	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	128	ARG
3	A	150	MET
3	A	154	THR
3	A	158	PRO
3	A	167	LEU
3	A	178	ASP
3	A	181	ILE
3	A	190	THR
3	A	191	PHE
3	A	194	LEU
3	A	195	ILE
3	A	200	GLN
3	A	206	LEU
3	A	219	CYS
3	A	226	ILE
3	A	233	GLU
3	B	4	LYS
3	B	9	GLN
3	B	16	ARG
3	B	17	ARG
3	B	27	ASN
3	B	44	GLN
3	B	64	LEU
3	B	69	LEU
3	B	98	ARG
3	B	101	TYR
3	B	103	TYR
3	B	115	SER
3	B	117	GLU
3	B	122	THR
3	B	125	ASP
3	B	129	TRP
3	B	130	VAL
3	B	132	THR
3	B	134	LYS
3	B	135	LYS
3	B	138	ASP
3	B	150	MET
3	B	151	THR
3	B	166	ILE
3	B	172	GLN
3	B	174	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	189	PHE
3	B	194	LEU
3	B	195	ILE
3	B	196	ARG
3	B	229	GLN
3	B	233	GLU
3	B	234	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	9	GLN
3	A	55	ASN
3	A	61	ASN
3	A	108	HIS
3	A	229	GLN
3	B	27	ASN
3	B	44	GLN
3	B	94	GLN
3	B	172	GLN
3	B	200	GLN
3	B	229	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	19/20 (95%)	-0.37	0 100 100	178, 189, 207, 213	0
2	D	19/20 (95%)	-0.11	0 100 100	182, 207, 222, 225	0
3	A	234/236 (99%)	-0.33	7 (2%) 50 38	95, 138, 187, 195	0
3	B	234/236 (99%)	-0.46	3 (1%) 77 68	83, 118, 170, 175	0
All	All	506/512 (98%)	-0.38	10 (1%) 65 55	83, 136, 195, 225	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	1	SER	4.0
3	B	4	LYS	3.6
3	A	1	SER	3.3
3	A	97	LEU	2.6
3	B	2	THR	2.5
3	A	4	LYS	2.3
3	A	119	ARG	2.1
3	A	120	THR	2.1
3	A	96	SER	2.1
3	A	122	THR	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.