



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:07 PM UTC

PDB ID : 5CRX / pdb_00005crx
Title : ASYMMETRIC DNA-BENDING IN THE CRE-LOXP SITE-SPECIFIC RE-COMBINATION SYNAPSE
Authors : Guo, F.; Gopaul, D.N.; Van Duyne, G.D.
Deposited on : 1999-04-21
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

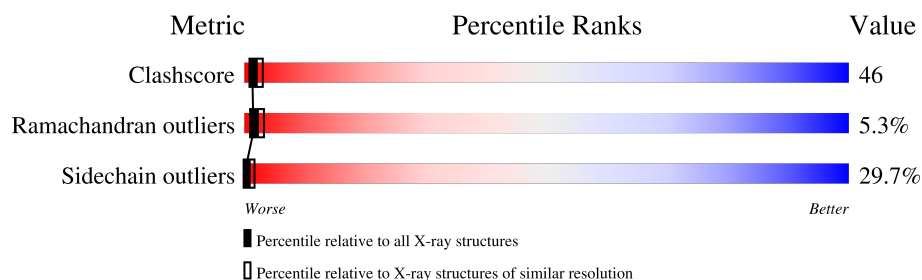
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	35	31% 60% • 6%
1	D	35	34% 57% • 6%
2	A	343	24% 39% 21% • 13%
2	B	343	32% 37% 16% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6364 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 (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	P	0	0	0
			677	325	122	197	33			
1	D	33	Total	C	N	O	P	0	0	0
			677	325	122	197	33			

- Molecule 2 is a protein called PROTEIN (BACTERIOPHAGE P1 CRE GENE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	297	Total	C	N	O	S	0	0	0
			2359	1462	452	431	14			
2	B	296	Total	C	N	O	S	0	0	0
			2337	1451	449	424	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	PHE	TYR	engineered mutation	UNP P06956
B	324	PHE	TYR	engineered mutation	UNP P06956

- Molecule 3 is water.

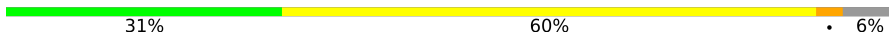
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	34	Total	O	0	0
			34	34		
3	D	56	Total	O	0	0
			56	56		
3	A	89	Total	O	0	0
			89	89		
3	B	135	Total	O	0	0
			135	135		

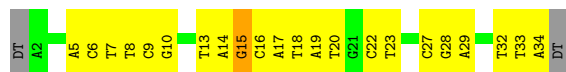
3 Residue-property plots [i](#)

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. 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. 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.

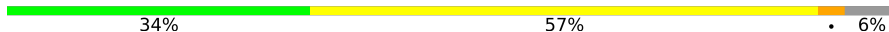
Note EDS was not executed.

• Molecule 1: DNA (35-MER)

Chain C: 



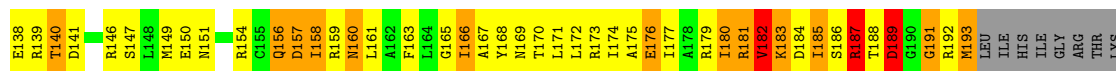
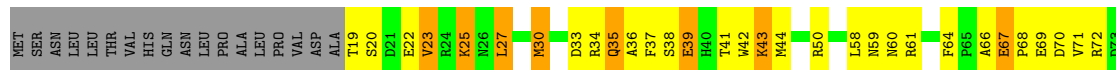
• Molecule 1: DNA (35-MER)

Chain D: 



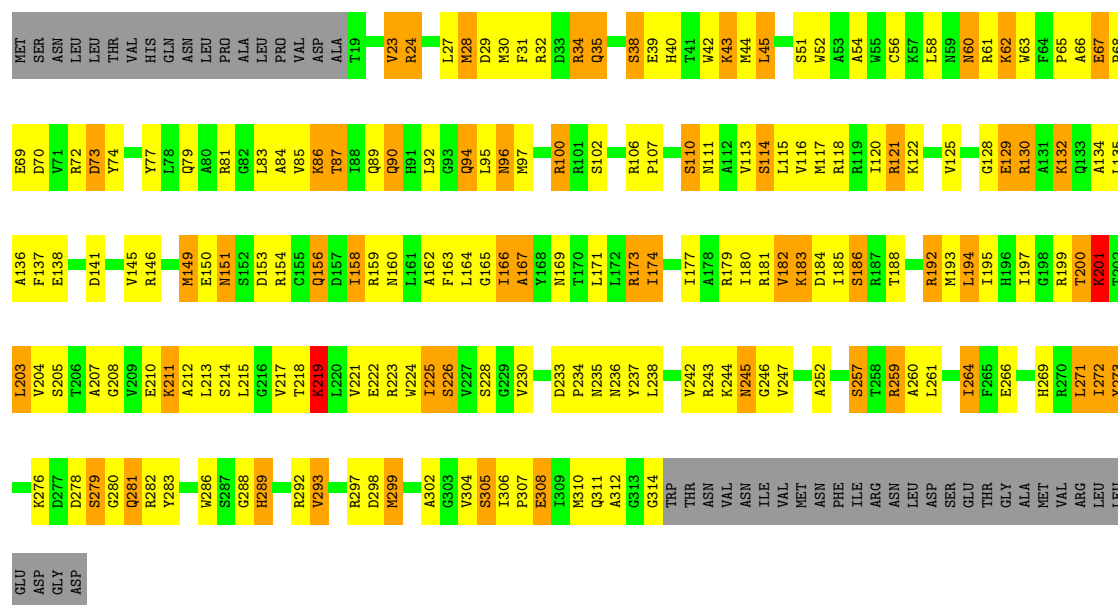
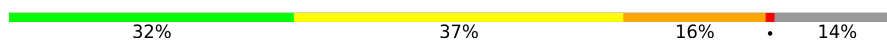
• Molecule 2: PROTEIN (BACTERIOPHAGE P1 CRE GENE)

Chain A: 



• Molecule 2: PROTEIN (BACTERIOPHAGE P1 CRE GENE)

Chain B:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.10Å 123.10Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.70	Depositor
% Data completeness (in resolution range)	96.1 (48.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.227 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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	C	0.42	0/759	0.82	0/1169
1	D	0.40	0/759	0.80	0/1169
2	A	0.60	0/2396	1.01	10/3224 (0.3%)
2	B	0.65	0/2375	1.06	13/3199 (0.4%)
All	All	0.58	0/6289	0.98	23/8761 (0.3%)

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	333	GLY	N-CA-C	7.70	120.49	111.63
2	A	100	ARG	N-CA-C	-7.37	103.25	111.28
2	B	67	GLU	CA-C-N	6.87	128.43	119.84
2	B	67	GLU	C-N-CA	6.87	128.43	119.84
2	B	219	LYS	N-CA-C	-6.73	103.86	111.07
2	A	216	GLY	N-CA-C	-6.73	106.02	114.16
2	A	218	THR	N-CA-C	-6.69	103.99	111.28
2	A	67	GLU	CA-C-N	6.41	127.85	119.84
2	A	67	GLU	C-N-CA	6.41	127.85	119.84
2	A	258	THR	N-CA-C	-6.07	104.67	111.28
2	B	272	ILE	CB-CA-C	-5.96	104.25	112.24
2	B	67	GLU	N-CA-C	-5.89	100.45	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	136	ALA	N-CA-C	5.87	118.78	110.50
2	B	207	ALA	N-CA-C	-5.79	105.23	112.93
2	B	174	ILE	N-CA-C	5.74	116.47	110.62
2	B	259	ARG	N-CA-C	-5.57	105.20	111.28
2	B	273	TYR	N-CA-C	5.42	119.87	112.88
2	B	182	VAL	N-CA-C	-5.41	104.29	111.05
2	A	116	VAL	CB-CA-C	-5.40	104.77	112.22
2	A	85	VAL	N-CA-C	-5.37	105.27	110.42
2	A	191	GLY	N-CA-C	-5.29	107.92	115.64
2	B	173	ARG	N-CA-C	-5.28	103.52	110.43
2	B	302	ALA	N-CA-C	-5.02	106.85	113.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	DG	Sidechain
1	D	17	DA	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	C	677	0	375	41	0
1	D	677	0	375	63	0
2	A	2359	0	2364	295	4
2	B	2337	0	2362	184	4
3	A	89	0	0	18	0
3	B	135	0	0	19	0
3	C	34	0	0	4	0
3	D	56	0	0	8	0
All	All	6364	0	5476	532	4

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 46.

All (532) 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:D:5:DA:H1'	1:D:6:DC:H5'	1.23	1.14
1:D:6:DC:H2''	1:D:7:DT:H71	1.26	1.12
2:B:181:ARG:HA	3:B:439:HOH:O	1.50	1.11
1:C:17:DA:H2''	1:C:18:DT:C5'	1.82	1.09
1:D:19:DA:H2''	1:D:20:DT:C5'	1.86	1.04
1:C:17:DA:H2''	1:C:18:DT:O5'	1.58	1.03
1:D:6:DC:H5''	3:D:64:HOH:O	1.56	1.03
2:A:166:ILE:HD11	2:A:177:ILE:HG23	1.40	1.02
2:A:232:ASP:HB2	3:A:418:HOH:O	1.59	1.01
2:A:185:ILE:HG22	2:A:193:MET:HB3	1.40	0.99
2:A:243:ARG:HH11	2:A:243:ARG:HG3	1.24	0.98
1:C:13:DT:OP2	2:B:87:THR:HG21	1.64	0.97
1:C:17:DA:H4'	3:C:48:HOH:O	1.63	0.96
2:A:133:GLN:HA	3:A:362:HOH:O	1.62	0.96
1:C:19:DA:H2''	1:C:20:DT:H5'	1.47	0.96
2:A:289:HIS:HB2	3:A:348:HOH:O	1.68	0.94
3:D:87:HOH:O	2:A:156:GLN:HG3	1.68	0.93
2:A:96:ASN:HD21	2:A:108:SER:HB2	1.34	0.93
2:A:259:ARG:HG3	2:A:259:ARG:HH11	1.34	0.91
1:D:18:DT:H3'	2:B:121:ARG:HE	1.34	0.90
1:C:17:DA:H2''	1:C:18:DT:H5''	1.51	0.89
1:D:24:DA:H5''	2:B:201:LYS:HB2	1.54	0.89
2:A:166:ILE:HG13	2:A:167:ALA:N	1.88	0.89
2:A:339:LEU:O	2:A:340:GLU:HG2	1.72	0.87
2:A:182:VAL:O	2:A:185:ILE:HG12	1.75	0.87
1:D:6:DC:C2'	1:D:7:DT:H71	2.04	0.87
2:B:205:SER:HB2	3:B:479:HOH:O	1.74	0.86
2:A:96:ASN:ND2	2:A:108:SER:HB2	1.89	0.85
1:D:14:DA:H5'	2:A:132:LYS:CE	2.06	0.85
2:A:177:ILE:O	2:A:180:ILE:HG23	1.76	0.85
2:A:193:MET:HG2	2:A:218:THR:HG23	1.58	0.84
1:D:14:DA:H5'	2:A:132:LYS:HE2	1.59	0.84
1:D:5:DA:C1'	1:D:6:DC:H5'	2.05	0.84
1:D:21:DG:H2''	1:D:22:DC:H5''	1.60	0.84
2:A:163:PHE:HE1	2:A:261:LEU:HD23	1.41	0.83
2:A:158:ILE:HG22	2:A:224:TRP:HB2	1.63	0.81
2:B:84:ALA:O	2:B:87:THR:HG23	1.79	0.81
2:A:172:LEU:HD21	2:A:211:LYS:HD3	1.62	0.81
1:C:5:DA:H2''	1:C:6:DC:H5''	1.62	0.81
2:B:182:VAL:HG23	2:B:236:ASN:O	1.81	0.80
2:A:156:GLN:HG2	2:A:157:ASP:N	1.95	0.80
2:B:141:ASP:O	2:B:145:VAL:HG23	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:ARG:HD2	2:A:106:ARG:HD3	1.64	0.79
1:D:5:DA:H1'	1:D:6:DC:C5'	2.10	0.79
2:A:170:THR:HB	2:A:172:LEU:HG	1.65	0.79
2:A:305:SER:OG	2:A:307:PRO:HD2	1.83	0.79
2:B:213:LEU:HB2	2:B:218:THR:HG22	1.64	0.78
2:A:121:ARG:O	2:A:125:VAL:HG23	1.84	0.78
3:D:64:HOH:O	2:A:241:ARG:HD3	1.82	0.77
1:D:18:DT:H3'	2:B:121:ARG:NE	1.99	0.77
2:B:181:ARG:HB2	2:B:184:ASP:OD2	1.85	0.76
1:D:22:DC:H2'	1:D:23:DT:H71	1.67	0.76
1:C:16:DC:H2''	1:C:17:DA:O5'	1.85	0.76
1:C:19:DA:H2''	1:C:20:DT:C5'	2.14	0.76
2:A:121:ARG:HH11	2:A:121:ARG:HB2	1.51	0.76
2:B:96:ASN:ND2	2:B:107:PRO:HD2	2.00	0.75
2:A:181:ARG:HA	2:A:237:TYR:HA	1.68	0.75
2:A:154:ARG:HB2	2:A:157:ASP:HB2	1.68	0.75
2:A:180:ILE:HG12	2:A:238:LEU:HB2	1.68	0.75
2:A:166:ILE:HD11	2:A:177:ILE:CG2	2.16	0.74
2:B:45:LEU:HA	2:B:94:GLN:CG	2.17	0.74
2:A:243:ARG:HH11	2:A:243:ARG:CG	2.00	0.74
1:D:24:DA:C5'	2:B:201:LYS:HB2	2.19	0.73
2:A:99:HIS:HB3	2:A:105:PRO:O	1.88	0.73
2:A:163:PHE:CE1	2:A:261:LEU:HD23	2.22	0.73
2:B:85:VAL:O	2:B:89:GLN:HG3	1.88	0.73
2:A:23:VAL:HG23	2:A:27:LEU:CD2	2.18	0.73
1:D:19:DA:H2''	1:D:20:DT:O5'	1.87	0.73
2:A:245:ASN:H	2:A:245:ASN:HD22	1.37	0.72
1:C:8:DT:H1'	1:C:9:DC:H5'	1.72	0.71
2:A:96:ASN:HD21	2:A:108:SER:CB	2.02	0.71
2:B:193:MET:HE2	2:B:222:GLU:HG3	1.73	0.71
2:A:23:VAL:O	2:A:27:LEU:HD22	1.91	0.71
2:A:170:THR:CB	2:A:172:LEU:HG	2.20	0.71
2:A:140:THR:OG1	3:A:386:HOH:O	2.09	0.71
2:B:269:HIS:CD2	3:B:372:HOH:O	2.43	0.71
2:A:133:GLN:N	3:A:417:HOH:O	2.23	0.70
1:C:5:DA:OP1	3:C:68:HOH:O	2.09	0.70
2:B:214:SER:O	2:B:218:THR:HG23	1.91	0.70
2:A:106:ARG:HB2	2:A:109:ASP:OD2	1.92	0.70
2:A:271:LEU:HD13	2:A:271:LEU:C	2.17	0.70
2:A:298:ASP:HA	2:A:301:ARG:HH11	1.56	0.70
2:B:181:ARG:HD2	2:B:183:LYS:HD3	1.71	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:DA:N7	3:D:67:HOH:O	2.24	0.69
1:D:17:DA:H8	1:D:17:DA:H5''	1.58	0.69
2:B:299:MET:HE1	2:B:312:ALA:HB2	1.74	0.69
1:C:10:DG:N7	3:C:69:HOH:O	2.25	0.69
1:D:7:DT:OP2	2:A:257:SER:HB3	1.91	0.69
2:A:174:ILE:HG13	2:A:175:ALA:H	1.58	0.68
2:B:283:TYR:HD2	3:B:371:HOH:O	1.75	0.68
1:D:19:DA:H1'	1:D:20:DT:OP1	1.93	0.68
2:A:81:ARG:HE	2:A:83:LEU:HD21	1.59	0.68
2:A:78:LEU:HA	2:A:81:ARG:HB2	1.75	0.68
1:C:7:DT:OP2	2:B:257:SER:HB3	1.95	0.67
2:A:59:ASN:O	2:A:61:ARG:HG2	1.93	0.67
2:A:269:HIS:HB2	2:A:286:TRP:CE3	2.29	0.67
2:A:130:ARG:HD3	3:A:374:HOH:O	1.94	0.67
1:C:17:DA:H2	1:D:20:DT:H3	1.39	0.67
1:D:17:DA:H5''	1:D:17:DA:C8	2.30	0.67
2:A:85:VAL:HG23	2:A:129:GLU:OE2	1.94	0.66
2:A:132:LYS:HB2	2:A:283:TYR:CE1	2.29	0.66
2:B:180:ILE:HG12	2:B:195:ILE:HG21	1.76	0.66
2:B:217:VAL:O	2:B:221:VAL:HG23	1.96	0.66
2:A:193:MET:CG	2:A:218:THR:HG23	2.25	0.66
2:A:298:ASP:HA	2:A:301:ARG:NH1	2.11	0.66
2:A:33:ASP:OD2	2:B:72:ARG:NH1	2.29	0.65
2:A:245:ASN:HD22	2:A:245:ASN:N	1.90	0.65
1:C:17:DA:C2'	1:C:18:DT:H5''	2.26	0.65
1:D:19:DA:H2''	1:D:20:DT:H5'	1.77	0.65
2:A:84:ALA:O	2:A:88:ILE:HG13	1.96	0.65
2:A:259:ARG:HG3	2:A:259:ARG:NH1	2.02	0.65
2:A:50:ARG:NH2	3:A:434:HOH:O	2.29	0.65
2:A:138:GLU:HG3	3:A:401:HOH:O	1.97	0.64
2:A:257:SER:O	2:A:261:LEU:HD12	1.97	0.64
1:C:28:DG:H2''	1:C:29:DA:O5'	1.98	0.64
2:A:58:LEU:HD23	2:A:59:ASN:HD21	1.62	0.64
2:A:185:ILE:CG2	2:A:193:MET:HB3	2.24	0.64
2:A:224:TRP:HA	2:A:227:VAL:HB	1.79	0.64
2:B:45:LEU:HA	2:B:94:GLN:HG2	1.79	0.64
2:B:183:LYS:HE3	2:B:235:ASN:ND2	2.12	0.64
2:A:134:ALA:HA	2:A:283:TYR:CD2	2.33	0.64
2:B:280:GLY:HA2	3:B:475:HOH:O	1.97	0.64
2:A:193:MET:CE	2:A:221:VAL:HB	2.28	0.63
2:A:271:LEU:CD1	2:A:272:ILE:HG13	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:258:THR:HA	2:A:261:LEU:HD13	1.78	0.63
2:B:138:GLU:HG2	2:B:298:ASP:OD2	1.98	0.63
1:D:5:DA:H5'	2:A:244:LYS:CA	2.27	0.63
2:A:217:VAL:O	2:A:221:VAL:HG23	1.98	0.63
2:A:339:LEU:O	2:A:340:GLU:CG	2.47	0.63
2:B:158:ILE:HD13	2:B:223:ARG:CZ	2.29	0.63
2:A:277:ASP:OD2	2:A:284:LEU:HD22	1.98	0.63
2:B:81:ARG:NH1	3:B:374:HOH:O	2.32	0.63
2:B:39:GLU:O	2:B:43:LYS:HD2	1.99	0.63
2:A:139:ARG:HB2	2:A:168:TYR:OH	1.99	0.62
2:A:174:ILE:HA	2:A:177:ILE:HD12	1.80	0.62
2:B:39:GLU:CD	2:B:39:GLU:H	2.07	0.62
2:A:282:ARG:O	2:A:283:TYR:HB2	2.00	0.62
2:A:119:ARG:HD2	2:A:123:GLU:CD	2.24	0.62
2:B:193:MET:H	2:B:218:THR:HG21	1.64	0.62
2:B:169:ASN:HD21	2:B:214:SER:H	1.46	0.62
2:B:171:LEU:O	2:B:292:ARG:HG3	1.99	0.62
2:A:166:ILE:HD11	2:A:177:ILE:HG12	1.80	0.62
2:A:249:ALA:H	2:A:250:PRO:HD3	1.65	0.62
2:B:96:ASN:HD22	2:B:107:PRO:HD2	1.65	0.62
1:D:5:DA:H5'	2:A:244:LYS:HA	1.82	0.61
2:A:174:ILE:HD12	2:A:258:THR:HB	1.81	0.61
1:D:5:DA:C5'	2:A:244:LYS:HA	2.30	0.61
2:A:146:ARG:O	2:A:150:GLU:HB2	2.00	0.61
2:A:181:ARG:HD2	2:A:236:ASN:O	2.00	0.61
2:A:174:ILE:HG13	2:A:175:ALA:N	2.16	0.61
2:A:160:ASN:N	2:A:160:ASN:HD22	1.97	0.61
2:B:67:GLU:OE2	2:B:68:PRO:HD2	2.01	0.61
2:B:132:LYS:NZ	3:B:393:HOH:O	2.34	0.61
2:B:181:ARG:NH1	2:B:235:ASN:O	2.33	0.61
2:A:307:PRO:O	2:A:311:GLN:N	2.33	0.61
2:A:193:MET:HE3	2:A:221:VAL:HB	1.83	0.60
2:A:261:LEU:HD12	2:A:261:LEU:H	1.66	0.60
2:A:25:LYS:NZ	2:B:69:GLU:OE1	2.34	0.60
2:A:132:LYS:HB2	2:A:283:TYR:HE1	1.64	0.60
2:A:158:ILE:CG2	2:A:224:TRP:HB2	2.31	0.60
2:A:182:VAL:HG23	2:A:236:ASN:H	1.66	0.60
1:D:19:DA:H2''	1:D:20:DT:H5''	1.81	0.60
2:B:180:ILE:HG12	2:B:195:ILE:CG2	2.31	0.60
2:A:156:GLN:HE21	2:A:156:GLN:H	1.48	0.60
1:D:24:DA:H4'	2:B:201:LYS:HD3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:DC:OP2	2:B:156:GLN:NE2	2.35	0.59
2:A:166:ILE:CD1	2:A:177:ILE:HG23	2.24	0.59
2:B:186:SER:O	2:B:194:LEU:N	2.34	0.59
2:A:30:MET:HE1	2:A:101:ARG:HG3	1.84	0.59
2:B:163:PHE:HD2	2:B:264:ILE:HG21	1.66	0.59
1:D:14:DA:C5'	2:A:132:LYS:HG3	2.32	0.59
2:A:176:GLU:HA	2:A:179:ARG:HD3	1.85	0.59
2:A:255:GLN:HB3	3:A:369:HOH:O	2.02	0.59
2:A:133:GLN:NE2	3:A:362:HOH:O	2.34	0.59
2:A:185:ILE:HD13	2:A:185:ILE:N	2.17	0.58
2:A:305:SER:HG	2:A:307:PRO:HD2	1.67	0.58
1:C:32:DT:H73	3:C:67:HOH:O	2.02	0.58
2:A:96:ASN:CG	2:A:108:SER:HB2	2.29	0.58
2:A:182:VAL:HG21	2:A:234:PRO:HA	1.86	0.58
2:B:306:ILE:HB	2:B:307:PRO:HD3	1.84	0.58
2:A:58:LEU:HD23	2:A:59:ASN:ND2	2.18	0.58
2:A:186:SER:O	2:A:188:THR:N	2.36	0.58
2:A:213:LEU:HD13	2:A:221:VAL:HG21	1.84	0.58
2:B:77:TYR:O	2:B:81:ARG:HG3	2.04	0.58
2:A:132:LYS:HD2	2:A:282:ARG:HD2	1.85	0.58
2:A:326:ARG:O	2:A:326:ARG:NE	2.37	0.58
2:B:150:GLU:HG2	2:B:151:ASN:N	2.19	0.58
1:D:20:DT:H2''	1:D:21:DG:O5'	2.04	0.58
2:A:326:ARG:NH2	2:A:331:GLU:O	2.36	0.58
2:B:193:MET:CE	2:B:222:GLU:HG3	2.33	0.58
2:B:224:TRP:CZ3	2:B:228:SER:HB3	2.38	0.58
2:B:245:ASN:HD22	2:B:247:VAL:CG2	2.17	0.58
1:D:18:DT:H5''	2:B:121:ARG:HH21	1.69	0.58
2:A:71:VAL:O	2:A:74:TYR:HB3	2.03	0.57
2:B:60:ASN:O	2:B:61:ARG:HD2	2.04	0.57
2:B:45:LEU:HA	2:B:94:GLN:HG3	1.84	0.57
2:A:304:VAL:HG12	2:A:305:SER:O	2.04	0.57
2:A:37:PHE:CZ	2:A:97:MET:HE2	2.38	0.57
2:B:205:SER:CB	3:B:479:HOH:O	2.40	0.57
1:D:14:DA:H5'	2:A:132:LYS:HE3	1.84	0.57
2:A:159:ARG:HH21	2:A:160:ASN:HD21	1.53	0.57
2:B:245:ASN:HD22	2:B:247:VAL:HG23	1.68	0.57
2:A:225:ILE:HG22	2:A:226:SER:N	2.18	0.57
2:B:181:ARG:CD	2:B:183:LYS:HD3	2.34	0.57
2:A:122:LYS:HG3	2:A:123:GLU:N	2.20	0.56
2:A:174:ILE:O	2:A:177:ILE:HB	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:271:LEU:HD22	2:A:271:LEU:O	2.05	0.56
2:A:306:ILE:N	2:A:307:PRO:CD	2.69	0.56
2:B:121:ARG:HH11	2:B:121:ARG:HB3	1.69	0.56
1:D:12:DA:OP1	2:A:81:ARG:NH2	2.37	0.56
2:A:64:PHE:CZ	2:A:104:LEU:HD11	2.40	0.56
2:A:74:TYR:O	2:A:77:TYR:HB3	2.04	0.56
2:A:271:LEU:HD13	2:A:272:ILE:HG13	1.88	0.56
2:B:23:VAL:HG22	2:B:102:SER:O	2.04	0.56
1:C:15:DG:H2''	1:C:16:DC:H5''	1.87	0.56
2:B:199:ARG:C	2:B:200:THR:HG22	2.31	0.56
2:B:188:THR:HG22	2:B:194:LEU:HD12	1.86	0.56
2:A:71:VAL:O	2:A:74:TYR:N	2.39	0.56
2:A:83:LEU:HD13	2:A:87:THR:HG21	1.88	0.56
2:A:213:LEU:CD1	2:A:221:VAL:HG21	2.36	0.55
2:A:83:LEU:N	2:A:83:LEU:HD23	2.21	0.55
2:B:169:ASN:ND2	2:B:217:VAL:HG21	2.21	0.55
1:C:17:DA:C2'	1:C:18:DT:O5'	2.39	0.55
2:A:234:PRO:O	2:A:235:ASN:ND2	2.40	0.55
2:B:34:ARG:HB3	2:B:42:TRP:CE2	2.41	0.55
2:A:176:GLU:HG3	2:A:179:ARG:NH1	2.21	0.55
2:A:182:VAL:CG2	2:A:236:ASN:HB2	2.36	0.55
2:A:248:ALA:O	2:A:249:ALA:HB2	2.06	0.55
2:A:172:LEU:HD21	2:A:211:LYS:CD	2.35	0.55
1:C:17:DA:N1	1:D:20:DT:O4	2.40	0.55
2:A:138:GLU:N	2:A:141:ASP:OD2	2.39	0.54
2:A:225:ILE:O	2:A:230:VAL:HG22	2.06	0.54
2:A:234:PRO:C	2:A:236:ASN:H	2.15	0.54
2:B:45:LEU:HD23	2:B:94:GLN:HG3	1.89	0.54
2:B:199:ARG:O	2:B:200:THR:HG22	2.06	0.54
2:A:71:VAL:O	2:A:72:ARG:C	2.50	0.54
2:A:112:ALA:O	2:A:116:VAL:HG22	2.07	0.54
2:A:122:LYS:CG	2:A:123:GLU:N	2.71	0.54
2:A:234:PRO:C	2:A:235:ASN:CG	2.75	0.54
2:B:134:ALA:HA	2:B:283:TYR:CD2	2.43	0.54
1:D:6:DC:H4'	2:A:241:ARG:HD3	1.89	0.54
2:A:23:VAL:HG23	2:A:27:LEU:HD21	1.89	0.54
2:A:96:ASN:ND2	2:A:108:SER:CB	2.65	0.54
2:A:159:ARG:HB2	2:A:224:TRP:CE3	2.43	0.54
1:C:33:DT:H2''	1:C:34:DA:C8	2.43	0.54
2:B:181:ARG:HG2	3:B:439:HOH:O	2.08	0.54
2:B:200:THR:O	2:B:201:LYS:C	2.50	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LYS:NZ	3:B:436:HOH:O	2.41	0.53
2:B:165:GLY:O	2:B:169:ASN:HB2	2.08	0.53
2:B:186:SER:O	2:B:194:LEU:HB2	2.08	0.53
1:C:5:DA:H4'	2:B:242:VAL:O	2.09	0.53
2:B:224:TRP:CH2	2:B:228:SER:HB3	2.43	0.53
2:A:77:TYR:HD1	3:A:392:HOH:O	1.90	0.53
1:C:5:DA:C2'	1:C:6:DC:H5''	2.34	0.53
2:A:30:MET:HG2	2:A:42:TRP:HH2	1.73	0.53
2:A:67:GLU:O	2:A:70:ASP:HB2	2.08	0.53
1:D:4:DA:O4'	2:A:244:LYS:HE3	2.08	0.53
2:A:156:GLN:HB3	2:A:242:VAL:HG11	1.91	0.53
2:B:244:LYS:C	2:B:246:GLY:H	2.15	0.53
2:A:33:ASP:CG	2:B:72:ARG:NH1	2.67	0.53
2:A:125:VAL:HG12	2:A:125:VAL:O	2.09	0.53
2:A:80:ALA:C	2:A:82:GLY:N	2.64	0.52
1:D:4:DA:H1'	2:A:244:LYS:HB2	1.91	0.52
2:B:257:SER:OG	2:B:259:ARG:HB3	2.09	0.52
2:B:107:PRO:O	2:B:113:VAL:HB	2.10	0.52
2:A:233:ASP:OD1	2:A:234:PRO:O	2.28	0.52
2:A:277:ASP:OD1	2:A:277:ASP:N	2.40	0.52
1:C:6:DC:H2''	1:C:7:DT:O5'	2.10	0.52
2:A:133:GLN:O	2:A:134:ALA:CB	2.57	0.52
2:A:310:MET:HG2	2:A:311:GLN:N	2.23	0.52
2:B:305:SER:CB	3:B:402:HOH:O	2.57	0.52
2:B:128:GLY:HA2	3:B:457:HOH:O	2.10	0.51
1:C:5:DA:C2	1:C:6:DC:C2	2.99	0.51
1:D:17:DA:H2'	1:D:18:DT:C6	2.45	0.51
1:D:33:DT:H2''	1:D:34:DA:N7	2.26	0.51
1:D:24:DA:C4'	2:B:201:LYS:HD3	2.39	0.51
2:A:137:PHE:O	2:A:294:GLY:HA3	2.09	0.51
2:A:245:ASN:H	2:A:245:ASN:ND2	2.08	0.51
2:B:181:ARG:O	2:B:184:ASP:HB2	2.10	0.51
2:A:76:LEU:HD21	2:A:116:VAL:HG12	1.91	0.51
2:B:156:GLN:HE21	2:B:159:ARG:NH2	2.09	0.51
2:A:166:ILE:CD1	2:A:177:ILE:HG12	2.41	0.51
2:A:182:VAL:HG23	2:A:236:ASN:N	2.25	0.51
2:B:305:SER:HB3	3:B:402:HOH:O	2.11	0.51
1:C:22:DC:H4'	2:B:118:ARG:NH2	2.25	0.51
1:D:5:DA:C2'	1:D:6:DC:H5'	2.40	0.51
2:A:126:ASP:OD1	2:A:126:ASP:N	2.44	0.51
2:A:185:ILE:HG21	2:A:193:MET:SD	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:282:ARG:HG3	2:A:282:ARG:HH11	1.76	0.51
2:B:278:ASP:OD2	2:B:279:SER:N	2.43	0.51
2:A:130:ARG:CD	3:A:374:HOH:O	2.54	0.51
2:A:177:ILE:O	2:A:180:ILE:CG2	2.54	0.51
2:B:160:ASN:O	2:B:164:LEU:HD12	2.11	0.51
1:C:13:DT:H2'	2:B:87:THR:HG22	1.93	0.50
2:B:77:TYR:CZ	2:B:81:ARG:HD3	2.45	0.50
2:B:169:ASN:HD22	2:B:217:VAL:HG21	1.76	0.50
2:B:233:ASP:OD1	2:B:234:PRO:HD2	2.12	0.50
1:D:23:DT:H3'	2:B:38:SER:HB2	1.93	0.50
1:D:2:DA:H2''	1:D:3:DT:O5'	2.11	0.50
2:A:295:ALA:O	2:A:299:MET:HB2	2.10	0.50
2:B:199:ARG:C	2:B:200:THR:CG2	2.84	0.50
2:A:234:PRO:C	2:A:236:ASN:N	2.69	0.50
1:C:32:DT:H2''	1:C:33:DT:OP2	2.12	0.50
2:B:154:ARG:HH21	2:B:156:GLN:HB3	1.76	0.50
2:A:139:ARG:HB2	2:A:168:TYR:HH	1.76	0.50
1:C:27:DC:H5''	2:A:282:ARG:HG2	1.94	0.50
2:A:39:GLU:HB2	2:A:43:LYS:NZ	2.27	0.50
2:A:163:PHE:HA	2:A:239:PHE:CZ	2.46	0.49
2:A:326:ARG:HH22	2:A:331:GLU:C	2.20	0.49
2:A:106:ARG:HB2	2:A:109:ASP:CG	2.37	0.49
2:A:171:LEU:HD12	2:A:171:LEU:N	2.28	0.49
2:A:232:ASP:O	2:A:234:PRO:HD3	2.12	0.49
2:A:261:LEU:HA	2:A:264:ILE:HD12	1.94	0.49
3:D:39:HOH:O	2:A:156:GLN:HB2	2.12	0.49
2:B:34:ARG:HB3	2:B:42:TRP:CZ2	2.48	0.49
2:B:137:PHE:HD1	2:B:286:TRP:CE2	2.30	0.49
2:A:174:ILE:O	2:A:177:ILE:N	2.45	0.49
2:A:33:ASP:OD1	2:B:72:ARG:NH1	2.43	0.49
2:A:124:ASN:O	2:A:129:GLU:HB2	2.13	0.49
3:D:79:HOH:O	2:A:244:LYS:HB3	2.13	0.49
2:A:166:ILE:CG1	2:A:167:ALA:N	2.71	0.49
2:A:187:ARG:HA	2:A:193:MET:HA	1.95	0.49
2:A:192:ARG:HA	2:A:218:THR:HG21	1.93	0.49
2:A:225:ILE:CG2	2:A:226:SER:N	2.75	0.49
2:B:193:MET:H	2:B:218:THR:CG2	2.25	0.49
2:B:205:SER:OG	2:B:208:GLY:HA2	2.13	0.49
2:A:282:ARG:HG3	2:A:282:ARG:NH1	2.28	0.48
2:B:269:HIS:HB2	2:B:286:TRP:CE3	2.47	0.48
2:A:119:ARG:O	2:A:123:GLU:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ASP:O	2:B:236:ASN:HB2	2.14	0.48
2:A:150:GLU:O	2:A:223:ARG:NH2	2.46	0.48
2:A:180:ILE:CG1	2:A:238:LEU:HB2	2.39	0.48
2:A:307:PRO:HA	2:A:310:MET:SD	2.53	0.48
1:C:23:DT:H73	2:A:41:THR:HG23	1.96	0.48
2:A:281:GLN:NE2	2:A:284:LEU:HD21	2.29	0.48
2:B:51:SER:O	2:B:54:ALA:HB3	2.13	0.48
2:B:183:LYS:HE3	2:B:235:ASN:HD21	1.77	0.48
2:B:282:ARG:NH2	3:B:474:HOH:O	2.46	0.48
2:B:306:ILE:HG22	2:B:310:MET:SD	2.53	0.48
2:B:166:ILE:HG22	2:B:167:ALA:N	2.27	0.48
2:B:179:ARG:NH2	2:B:199:ARG:HG2	2.29	0.48
2:B:219:LYS:HA	2:B:219:LYS:HE3	1.96	0.48
2:A:35:GLN:HB2	3:A:399:HOH:O	2.13	0.48
2:B:67:GLU:CD	2:B:68:PRO:HD2	2.39	0.48
2:B:181:ARG:CB	2:B:183:LYS:HG2	2.44	0.48
2:B:235:ASN:O	2:B:252:ALA:CB	2.62	0.47
2:A:36:ALA:O	2:B:118:ARG:NH1	2.47	0.47
2:A:133:GLN:O	2:A:134:ALA:HB2	2.12	0.47
2:A:249:ALA:N	2:A:250:PRO:HD3	2.29	0.47
2:B:56:CYS:SG	2:B:63:TRP:HA	2.54	0.47
2:B:203:LEU:HD21	2:B:208:GLY:HA2	1.95	0.47
1:D:5:DA:H5'	2:A:244:LYS:HB2	1.94	0.47
2:A:66:ALA:H	2:A:99:HIS:HE1	1.62	0.47
2:A:119:ARG:HG3	2:A:120:ILE:N	2.25	0.47
2:A:236:ASN:HA	2:A:251:SER:O	2.15	0.47
2:B:237:TYR:HB2	3:B:399:HOH:O	2.14	0.47
1:D:14:DA:H5'	2:A:132:LYS:HG3	1.96	0.47
2:B:31:PHE:O	2:B:34:ARG:HG2	2.14	0.47
2:B:74:TYR:O	2:B:77:TYR:HB3	2.14	0.47
2:B:188:THR:HG22	2:B:194:LEU:CD1	2.44	0.47
2:B:62:LYS:HD3	2:B:65:PRO:O	2.15	0.47
2:B:79:GLN:NE2	2:B:120:ILE:HG12	2.30	0.47
2:B:310:MET:O	2:B:314:GLY:N	2.45	0.47
1:D:20:DT:H5'	1:D:20:DT:H6	1.80	0.47
2:A:174:ILE:O	2:A:175:ALA:C	2.58	0.47
2:A:189:ASP:C	2:A:191:GLY:H	2.23	0.47
2:A:192:ARG:HD3	2:A:215:LEU:HG	1.97	0.47
1:D:19:DA:OP1	2:B:121:ARG:CZ	2.63	0.47
2:B:173:ARG:HG2	2:B:289:HIS:HE1	1.80	0.46
1:D:28:DG:N7	2:B:259:ARG:NH2	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:GLU:H	2:A:39:GLU:HG3	1.42	0.46
2:A:121:ARG:HH11	2:A:121:ARG:CB	2.26	0.46
2:A:326:ARG:NH2	2:A:331:GLU:C	2.73	0.46
1:C:17:DA:H5''	1:C:17:DA:H8	1.79	0.46
2:B:174:ILE:HA	2:B:177:ILE:HD12	1.98	0.46
2:A:158:ILE:HG13	3:A:412:HOH:O	2.16	0.46
2:A:158:ILE:O	2:A:159:ARG:C	2.57	0.46
2:B:28:MET:O	2:B:32:ARG:HB2	2.16	0.46
2:B:156:GLN:NE2	2:B:159:ARG:NH2	2.63	0.46
1:D:5:DA:H5'	2:A:244:LYS:CB	2.45	0.46
2:A:271:LEU:C	2:A:271:LEU:CD1	2.88	0.46
2:A:44:MET:HE3	2:A:44:MET:HA	1.98	0.46
2:A:80:ALA:C	2:A:82:GLY:H	2.23	0.46
2:A:146:ARG:O	2:A:150:GLU:CB	2.64	0.46
2:A:334:ALA:O	2:A:337:ARG:N	2.49	0.46
2:B:44:MET:HB3	2:B:90:GLN:HE22	1.81	0.46
2:B:228:SER:OG	2:B:230:VAL:HG22	2.16	0.46
2:A:181:ARG:HD3	2:A:237:TYR:CE2	2.51	0.45
1:C:17:DA:H5''	1:C:17:DA:C8	2.51	0.45
2:A:137:PHE:HB2	2:A:290:SER:HB3	1.98	0.45
2:A:271:LEU:HD13	2:A:271:LEU:O	2.16	0.45
2:A:339:LEU:O	2:A:340:GLU:CB	2.63	0.45
2:B:257:SER:O	2:B:260:ALA:HB3	2.17	0.45
1:C:17:DA:C2	1:D:21:DG:N2	2.84	0.45
2:A:174:ILE:HD12	2:A:258:THR:CB	2.45	0.45
2:B:135:LEU:HD21	3:B:372:HOH:O	2.16	0.45
2:B:305:SER:OG	2:B:307:PRO:HD2	2.16	0.45
2:B:304:VAL:CG1	2:B:305:SER:N	2.80	0.45
1:D:5:DA:H5''	2:A:244:LYS:HA	1.99	0.45
2:A:92:LEU:HD11	2:A:113:VAL:CG1	2.47	0.45
2:A:326:ARG:CZ	2:A:331:GLU:HB2	2.46	0.45
2:B:293:VAL:O	2:B:297:ARG:HG3	2.16	0.45
2:B:122:LYS:CE	3:B:436:HOH:O	2.65	0.44
2:B:181:ARG:O	2:B:184:ASP:N	2.48	0.44
1:D:17:DA:H2'	1:D:18:DT:C5	2.53	0.44
2:A:60:ASN:C	2:A:61:ARG:HG2	2.43	0.44
2:A:174:ILE:HD12	2:A:258:THR:CG2	2.47	0.44
2:A:236:ASN:HB3	2:A:237:TYR:H	1.63	0.44
1:D:22:DC:H2''	1:D:23:DT:C6	2.52	0.44
2:A:133:GLN:CB	3:A:417:HOH:O	2.64	0.44
2:A:176:GLU:HG3	2:A:179:ARG:HH11	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ARG:C	2:B:102:SER:H	2.25	0.44
2:A:72:ARG:HG3	2:A:116:VAL:HG11	1.99	0.44
2:A:170:THR:OG1	2:A:172:LEU:HG	2.16	0.44
2:A:289:HIS:O	2:A:290:SER:C	2.60	0.44
2:B:166:ILE:O	2:B:167:ALA:C	2.60	0.44
2:B:299:MET:HE1	2:B:312:ALA:CB	2.46	0.44
2:A:39:GLU:O	2:A:43:LYS:HD3	2.17	0.44
2:A:66:ALA:H	2:A:99:HIS:CE1	2.36	0.44
2:B:122:LYS:HE3	3:B:436:HOH:O	2.18	0.44
2:B:272:ILE:HB	2:B:273:TYR:CD1	2.53	0.44
1:D:18:DT:H2''	1:D:19:DA:OP2	2.17	0.44
2:A:33:ASP:CG	2:B:72:ARG:HH12	2.22	0.44
2:B:304:VAL:HG12	2:B:305:SER:N	2.33	0.44
2:A:172:LEU:HD21	2:A:211:LYS:HE3	1.99	0.44
2:A:192:ARG:HD3	2:A:214:SER:O	2.17	0.44
2:A:132:LYS:CD	2:A:282:ARG:HD2	2.48	0.43
2:A:243:ARG:HG3	2:A:243:ARG:NH1	2.05	0.43
2:A:257:SER:O	2:A:261:LEU:CD1	2.66	0.43
1:D:11:DT:H2''	1:D:12:DA:OP2	2.17	0.43
2:A:176:GLU:O	2:A:180:ILE:HG22	2.18	0.43
2:B:52:TRP:CZ2	2:B:66:ALA:HB2	2.53	0.43
2:B:113:VAL:O	2:B:116:VAL:HG12	2.19	0.43
1:D:22:DC:OP2	2:B:100:ARG:NH2	2.51	0.43
2:A:237:TYR:O	2:A:238:LEU:C	2.61	0.43
2:A:238:LEU:HD23	2:A:238:LEU:HA	1.74	0.43
2:A:243:ARG:HB2	2:A:245:ASN:HD21	1.84	0.43
2:B:306:ILE:CG2	2:B:310:MET:SD	3.06	0.43
2:A:219:LYS:HA	2:A:222:GLU:OE1	2.19	0.43
2:A:265:PHE:HZ	2:A:291:ALA:HB2	1.83	0.43
2:A:295:ALA:O	2:A:296:ALA:C	2.62	0.43
2:A:182:VAL:CG2	2:A:236:ASN:H	2.29	0.43
2:A:248:ALA:O	2:A:249:ALA:CB	2.67	0.43
2:B:70:ASP:HA	2:B:73:ASP:OD2	2.19	0.43
2:B:118:ARG:O	2:B:122:LYS:HG3	2.19	0.43
2:A:170:THR:O	2:A:171:LEU:C	2.62	0.43
2:A:187:ARG:HG3	2:A:191:GLY:O	2.19	0.43
2:A:224:TRP:O	2:A:225:ILE:C	2.60	0.43
2:A:289:HIS:C	2:A:291:ALA:N	2.74	0.43
2:B:92:LEU:O	2:B:92:LEU:HD12	2.19	0.43
2:B:179:ARG:NH2	3:B:384:HOH:O	2.45	0.43
1:C:22:DC:H5''	2:A:37:PHE:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:138:GLU:O	2:A:141:ASP:HB2	2.19	0.43
2:A:277:ASP:HB2	2:A:284:LEU:HD13	1.99	0.43
2:A:304:VAL:CG1	2:A:308:GLU:HB2	2.49	0.43
2:B:110:SER:O	2:B:114:SER:OG	2.33	0.43
2:B:225:ILE:HG22	2:B:226:SER:N	2.33	0.43
2:B:261:LEU:HA	2:B:264:ILE:CD1	2.49	0.43
2:A:244:LYS:O	2:A:244:LYS:HG2	2.15	0.42
2:A:306:ILE:N	2:A:307:PRO:HD3	2.33	0.42
2:A:330:SER:O	2:A:332:THR:N	2.49	0.42
2:B:177:ILE:HA	2:B:180:ILE:HD12	2.01	0.42
2:A:259:ARG:NH1	2:A:259:ARG:CG	2.74	0.42
2:B:23:VAL:HG12	2:B:24:ARG:N	2.32	0.42
1:D:24:DA:H5''	2:B:201:LYS:CB	2.39	0.42
2:A:179:ARG:NH2	3:A:383:HOH:O	2.52	0.42
2:B:116:VAL:CG1	2:B:117:MET:N	2.82	0.42
2:B:146:ARG:O	2:B:150:GLU:HB3	2.19	0.42
2:B:213:LEU:CB	2:B:218:THR:HG22	2.43	0.42
2:A:259:ARG:HH11	2:A:259:ARG:CG	2.15	0.42
2:B:85:VAL:HG23	2:B:129:GLU:OE2	2.18	0.42
2:A:96:ASN:OD1	2:A:108:SER:HB2	2.20	0.42
1:C:15:DG:C2'	1:C:16:DC:H5''	2.48	0.42
2:A:97:MET:O	2:A:101:ARG:HG2	2.20	0.42
2:A:104:LEU:H	2:A:104:LEU:HG	1.57	0.42
2:B:122:LYS:HE3	2:B:122:LYS:HB3	1.86	0.42
2:B:159:ARG:O	2:B:162:ALA:N	2.52	0.42
2:B:192:ARG:NH1	2:B:215:LEU:HG	2.34	0.42
2:B:197:ILE:CD1	2:B:211:LYS:HG3	2.49	0.42
1:D:20:DT:C4	1:D:21:DG:C6	3.08	0.42
2:A:69:GLU:OE1	2:A:72:ARG:HD3	2.19	0.42
2:A:80:ALA:O	2:A:82:GLY:N	2.53	0.42
2:A:182:VAL:CG2	2:A:234:PRO:HA	2.49	0.42
2:A:243:ARG:CG	2:A:243:ARG:NH1	2.68	0.42
2:B:185:ILE:HD11	2:B:238:LEU:HD13	2.01	0.42
2:B:244:LYS:C	2:B:246:GLY:N	2.77	0.42
2:A:102:SER:HB2	2:A:104:LEU:HD12	2.02	0.42
2:A:270:ARG:HG3	2:A:275:ALA:HA	2.02	0.42
2:A:291:ALA:O	2:A:292:ARG:C	2.62	0.42
2:A:306:ILE:H	2:A:307:PRO:HD3	1.85	0.42
1:D:3:DT:H3'	3:D:84:HOH:O	2.19	0.41
1:D:24:DA:H2''	1:D:25:DT:C7	2.49	0.41
2:A:243:ARG:CB	2:A:245:ASN:ND2	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ARG:HB2	2:B:183:LYS:HG2	2.02	0.41
2:A:185:ILE:CG2	2:A:193:MET:SD	3.07	0.41
2:B:235:ASN:O	2:B:252:ALA:HB1	2.19	0.41
2:A:89:GLN:HG3	2:A:117:MET:HE2	2.00	0.41
2:A:193:MET:HG2	2:A:193:MET:H	1.59	0.41
2:B:271:LEU:HD23	2:B:272:ILE:CD1	2.51	0.41
2:B:52:TRP:C	2:B:54:ALA:N	2.77	0.41
2:B:171:LEU:O	2:B:292:ARG:NH1	2.53	0.41
1:C:6:DC:H2''	1:C:7:DT:C5'	2.50	0.41
1:D:14:DA:H2'	3:D:46:HOH:O	2.21	0.41
1:C:14:DA:N7	2:B:86:LYS:HD3	2.36	0.41
2:A:149:MET:HE2	3:A:420:HOH:O	2.21	0.41
2:A:22:GLU:OE2	3:A:409:HOH:O	2.21	0.41
2:A:170:THR:C	2:A:172:LEU:N	2.77	0.41
2:A:231:ALA:O	2:A:232:ASP:O	2.39	0.41
1:C:14:DA:C8	2:B:86:LYS:HD3	2.56	0.41
2:A:80:ALA:O	2:A:81:ARG:C	2.64	0.41
2:A:170:THR:C	2:A:171:LEU:HD12	2.46	0.41
2:B:29:ASP:O	2:B:32:ARG:HB3	2.20	0.41
2:B:111:ASN:O	2:B:115:LEU:HD12	2.20	0.41
2:B:149:MET:HE2	2:B:149:MET:HB3	1.74	0.41
2:B:308:GLU:O	2:B:311:GLN:HB3	2.20	0.41
2:A:233:ASP:C	2:A:234:PRO:O	2.61	0.41
2:B:181:ARG:HB3	2:B:183:LYS:HG2	2.02	0.41
2:A:165:GLY:O	2:A:169:ASN:HB2	2.20	0.40
2:B:40:HIS:HA	2:B:43:LYS:HB2	2.03	0.40
2:B:130:ARG:N	2:B:130:ARG:HD2	2.36	0.40
1:D:5:DA:H4'	2:A:242:VAL:O	2.21	0.40
1:D:18:DT:C5'	2:B:121:ARG:HH21	2.34	0.40
2:A:223:ARG:O	2:A:227:VAL:HG23	2.21	0.40
2:B:128:GLY:O	2:B:130:ARG:HG3	2.21	0.40
2:B:138:GLU:N	2:B:141:ASP:OD2	2.53	0.40
1:C:22:DC:H5''	2:A:37:PHE:HE2	1.87	0.40
1:C:18:DT:H2''	1:C:19:DA:C8	2.57	0.40
2:A:270:ARG:CZ	2:A:270:ARG:HB3	2.50	0.40
2:A:278:ASP:O	2:A:279:SER:C	2.63	0.40
2:A:245:ASN:ND2	2:A:247:VAL:H	2.20	0.40
2:A:259:ARG:O	2:A:260:ALA:C	2.63	0.40
2:A:326:ARG:HE	2:A:329:ASP:HB2	1.87	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:332:THR:CG2	2:B:212:ALA:CB[4_566]	1.81	0.39
2:A:337:ARG:NH1	2:B:308:GLU:OE2[4_566]	2.04	0.16
2:A:122:LYS:CD	2:B:35:GLN:O[4_566]	2.06	0.14
2:A:327:ASN:ND2	2:B:194:LEU:CD2[4_566]	2.10	0.10

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	
2	A	291/343 (85%)	216 (74%)	49 (17%)	26 (9%)	0	0
2	B	294/343 (86%)	261 (89%)	28 (10%)	5 (2%)	7	19
All	All	585/686 (85%)	477 (82%)	77 (13%)	31 (5%)	1	3

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	134	ALA
2	A	214	SER
2	A	232	ASP
2	A	248	ALA
2	A	249	ALA
2	B	279	SER
2	A	20	SER
2	A	182	VAL
2	A	187	ARG
2	A	215	LEU
2	A	243	ARG
2	A	276	LYS
2	A	281	GLN
2	A	283	TYR
2	B	281	GLN
2	A	105	PRO
2	A	183	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	167	ALA
2	A	236	ASN
2	A	290	SER
2	A	329	ASP
2	B	288	GLY
2	A	278	ASP
2	A	279	SER
2	A	189	ASP
2	A	297	ARG
2	B	201	LYS
2	A	68	PRO
2	A	128	GLY
2	A	314	GLY
2	A	234	PRO

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	
2	A	247/287 (86%)	164 (66%)	83 (34%)	0	0
2	B	245/287 (85%)	182 (74%)	63 (26%)	0	2
All	All	492/574 (86%)	346 (70%)	146 (30%)	0	1

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	19	THR
2	A	23	VAL
2	A	25	LYS
2	A	27	LEU
2	A	30	MET
2	A	34	ARG
2	A	35	GLN
2	A	38	SER
2	A	39	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	43	LYS
2	A	81	ARG
2	A	83	LEU
2	A	86	LYS
2	A	90	GLN
2	A	92	LEU
2	A	95	LEU
2	A	97	MET
2	A	100	ARG
2	A	104	LEU
2	A	108	SER
2	A	116	VAL
2	A	118	ARG
2	A	119	ARG
2	A	121	ARG
2	A	126	ASP
2	A	129	GLU
2	A	130	ARG
2	A	132	LYS
2	A	140	THR
2	A	147	SER
2	A	151	ASN
2	A	156	GLN
2	A	157	ASP
2	A	158	ILE
2	A	160	ASN
2	A	161	LEU
2	A	166	ILE
2	A	173	ARG
2	A	176	GLU
2	A	180	ILE
2	A	181	ARG
2	A	182	VAL
2	A	183	LYS
2	A	184	ASP
2	A	185	ILE
2	A	187	ARG
2	A	189	ASP
2	A	193	MET
2	A	211	LYS
2	A	214	SER
2	A	215	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	219	LYS
2	A	223	ARG
2	A	224	TRP
2	A	225	ILE
2	A	235	ASN
2	A	238	LEU
2	A	241	ARG
2	A	243	ARG
2	A	244	LYS
2	A	245	ASN
2	A	253	THR
2	A	255	GLN
2	A	256	LEU
2	A	258	THR
2	A	259	ARG
2	A	271	LEU
2	A	276	LYS
2	A	277	ASP
2	A	281	GLN
2	A	282	ARG
2	A	298	ASP
2	A	301	ARG
2	A	308	GLU
2	A	309	ILE
2	A	310	MET
2	A	311	GLN
2	A	316	THR
2	A	326	ARG
2	A	328	LEU
2	A	332	THR
2	A	338	LEU
2	A	339	LEU
2	B	23	VAL
2	B	24	ARG
2	B	27	LEU
2	B	28	MET
2	B	30	MET
2	B	34	ARG
2	B	35	GLN
2	B	38	SER
2	B	43	LYS
2	B	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	58	LEU
2	B	60	ASN
2	B	62	LYS
2	B	73	ASP
2	B	83	LEU
2	B	86	LYS
2	B	87	THR
2	B	90	GLN
2	B	94	GLN
2	B	95	LEU
2	B	96	ASN
2	B	97	MET
2	B	100	ARG
2	B	106	ARG
2	B	110	SER
2	B	114	SER
2	B	121	ARG
2	B	125	VAL
2	B	129	GLU
2	B	130	ARG
2	B	132	LYS
2	B	149	MET
2	B	151	ASN
2	B	153	ASP
2	B	156	GLN
2	B	158	ILE
2	B	166	ILE
2	B	183	LYS
2	B	186	SER
2	B	192	ARG
2	B	194	LEU
2	B	200	THR
2	B	201	LYS
2	B	203	LEU
2	B	204	VAL
2	B	210	GLU
2	B	211	LYS
2	B	219	LYS
2	B	225	ILE
2	B	226	SER
2	B	243	ARG
2	B	245	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	257	SER
2	B	264	ILE
2	B	266	GLU
2	B	271	LEU
2	B	276	LYS
2	B	281	GLN
2	B	289	HIS
2	B	293	VAL
2	B	299	MET
2	B	305	SER
2	B	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	59	ASN
2	A	90	GLN
2	A	94	GLN
2	A	99	HIS
2	A	133	GLN
2	A	156	GLN
2	A	160	ASN
2	A	235	ASN
2	A	245	ASN
2	A	281	GLN
2	A	311	GLN
2	B	60	ASN
2	B	90	GLN
2	B	94	GLN
2	B	169	ASN
2	B	245	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 [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.