



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:32 PM GMT

PDB ID : 5CRX
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

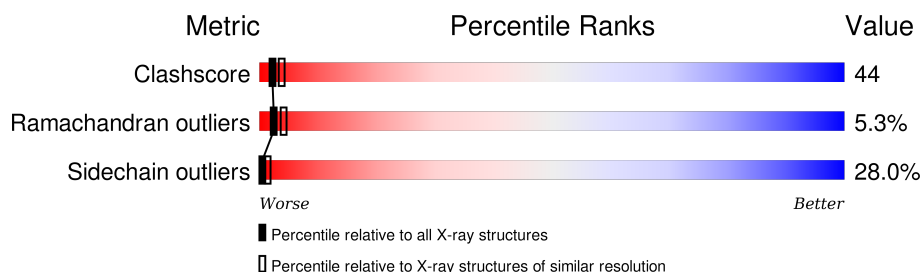
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	35	
1	D	35	
2	A	343	
2	B	343	

2 Entry composition [i](#)

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	UNP P06956
B	324	PHE	TYR	ENGINEERED	UNP P06956

- Molecule 3 is water.

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

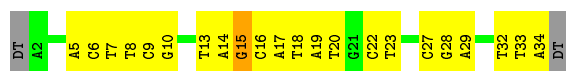
3 Residue-property plots [i](#)

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

Note EDS was not executed.

- Molecule 1: DNA (35-MER)

Chain C: 




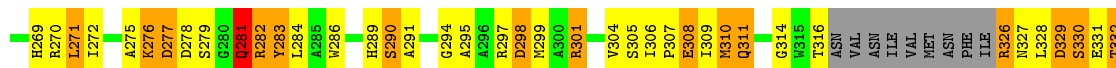
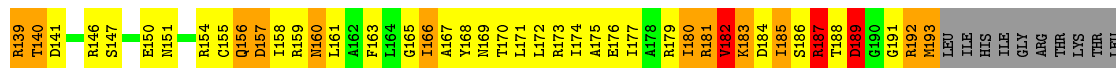
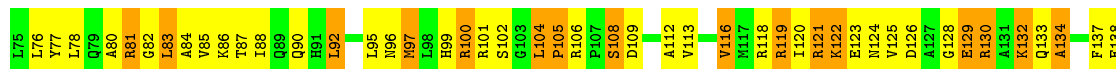
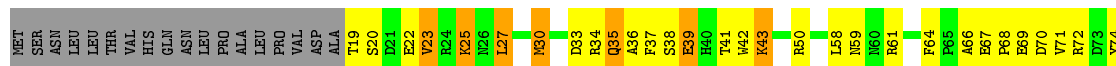
- Molecule 1: DNA (35-MER)

Chain D: 

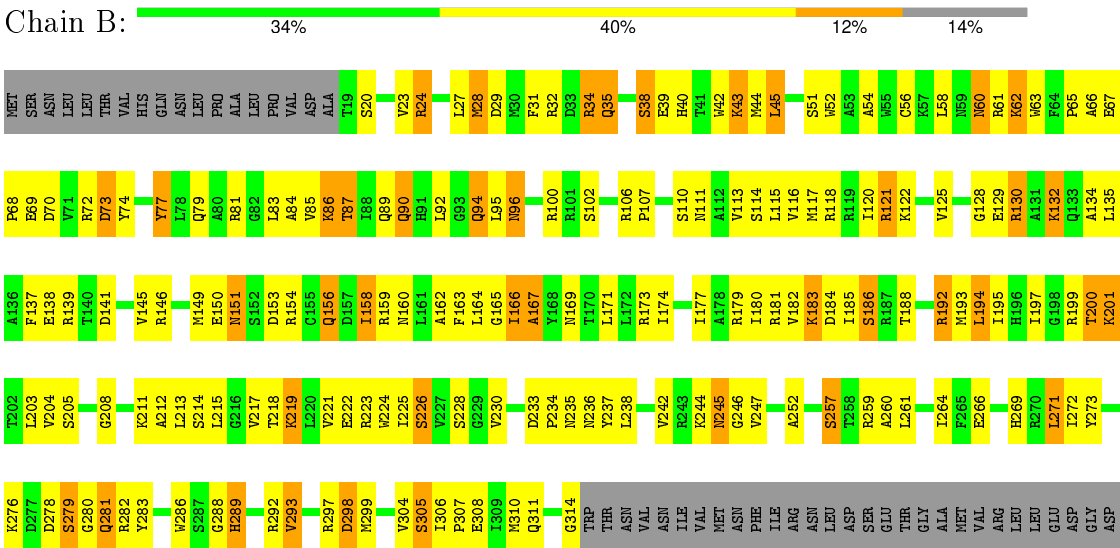


- Molecule 2: PROTEIN (BACTERIOPHAGE P1 CRE GENE)

Chain A: 



- Molecule 2: PROTEIN (BACTERIOPHAGE P1 CRE GENE)



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.10 Å 123.10 Å 180.00 Å 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	0.64	0/759	0.84	0/1169
1	D	0.62	0/759	0.83	0/1169
2	A	0.47	0/2396	0.66	0/3224
2	B	0.48	0/2375	0.68	0/3199
All	All	0.52	0/6289	0.72	0/8761

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.

There are no bond angle outliers.

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 [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	677	0	375	41	0
1	D	677	0	375	67	0
2	A	2359	0	2364	275	4
2	B	2337	0	2362	175	4
3	A	89	0	0	17	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	508	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 44.

All (508) 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
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:D:6:DC:H5''	3:D:64:HOH:O	1.56	1.03
1:C:17:DA:H2''	1:C:18:DT:O5'	1.58	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:HG3	2:A:243:ARG:HH11	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:84:ALA:O	2:B:87:THR:HG23	1.79	0.81
2:A:158:ILE:HG22	2:A:224:TRP:HB2	1.63	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
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: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:HB2	2:A:121:ARG:HH11	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:CG	2:A:243:ARG:HH11	2.00	0.74
1:D:24:DA:C5'	2:B:201:LYS:HB2	2.19	0.73
2:A:163:PHE:CE1	2:A:261:LEU:HD23	2.22	0.73
2:A:99:HIS:HB3	2:A:105:PRO:O	1.88	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:96:ASN:HD21	2:A:108:SER:CB	2.02	0.71
1:D:6:DC:H2''	1:D:7:DT:C7	2.21	0.71
2:A:170:THR:CB	2:A:172:LEU:HG	2.20	0.71
2:A:23:VAL:O	2:A:27:LEU:HD22	1.91	0.71
2:B:269:HIS:CD2	3:B:372:HOH:O	2.43	0.71
2:A:140:THR:OG1	3:A:386:HOH:O	2.09	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: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
1:D:4:DA:N7	3:D:67:HOH:O	2.24	0.69
1:D:17:DA:H5''	1:D:17:DA:H8	1.58	0.69
1:D:7:DT:OP2	2:A:257:SER:HB3	1.91	0.69
1:C:10:DG:N7	3:C:69:HOH:O	2.25	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:D:6:DC:C2'	1:D:7:DT:H72	2.25	0.67
1:C:7:DT:OP2	2:B:257:SER:HB3	1.95	0.67
2:A:269:HIS:HB2	2:A:286:TRP:CE3	2.29	0.67
2:A:59:ASN:O	2:A:61:ARG:HG2	1.93	0.67
2:A:130:ARG:HD3	3:A:374:HOH:O	1.94	0.67
1:D:17:DA:H5''	1:D:17:DA:C8	2.30	0.67
1:C:17:DA:H2	1:D:20:DT:H3	1.39	0.67
2:A:132:LYS:HB2	2:A:283:TYR:CE1	2.29	0.66
2:A:85:VAL:HG23	2:A:129:GLU:OE2	1.94	0.66
2:B:217:VAL:O	2:B:221:VAL:HG23	1.96	0.66
2:B:180:ILE:HG12	2:B:195:ILE:HG21	1.76	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:245:ASN:N	2:A:245:ASN:HD22	1.90	0.65
2:A:33:ASP:OD2	2:B:72:ARG:NH1	2.29	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:B:193:MET:HE2	2:B:222:GLU:HG3	1.78	0.65
2:A:259:ARG:HG3	2:A:259:ARG:NH1	2.02	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:271:LEU:HD13	2:A:271:LEU:C	2.17	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
2:A:58:LEU:HD23	2:A:59:ASN:HD21	1.62	0.64
1:C:28:DG:H2''	1:C:29:DA:O5'	1.98	0.64
2:B:183:LYS:HE3	2:B:235:ASN:ND2	2.12	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
1:D:6:DC:H2''	1:D:7:DT:H72	1.79	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
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:174:ILE:HA	2:A:177:ILE:HD12	1.80	0.62
2:A:139:ARG:HB2	2:A:168:TYR:OH	1.99	0.62
2:A:282:ARG:O	2:A:283:TYR:HB2	2.00	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:B:96:ASN:HD22	2:B:107:PRO:HD2	1.65	0.62
2:A:249:ALA:H	2:A:250:PRO:HD3	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:181:ARG:HD2	2:A:236:ASN:O	2.00	0.61
2:A:146:ARG:O	2:A:150:GLU:HB2	2.00	0.61
2:A:174:ILE:HG13	2:A:175:ALA:N	2.16	0.61
2:A:160:ASN:HD22	2:A:160:ASN:N	1.97	0.61
2:B:181:ARG:NH1	2:B:235:ASN:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:GLU:OE2	2:B:68:PRO:HD2	2.01	0.61
2:A:307:PRO:O	2:A:311:GLN:N	2.33	0.61
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:182:VAL:HG23	2:A:236:ASN:H	1.66	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:193:MET:HE3	2:A:221:VAL:HB	1.84	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
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:B:163:PHE:HD2	2:B:264:ILE:HG21	1.66	0.59
2:A:176:GLU:HA	2:A:179:ARG:HD3	1.85	0.59
1:D:14:DA:C5'	2:A:132:LYS:HG3	2.32	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:119:ARG:HD2	2:A:123:GLU:CD	2.24	0.59
2:A:185:ILE:N	2:A:185:ILE:HD13	2.17	0.58
1:C:32:DT:H73	3:C:67:HOH:O	2.02	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:213:LEU:HD13	2:A:221:VAL:HG21	1.84	0.58
2:A:58:LEU:HD23	2:A:59:ASN:ND2	2.18	0.58
2:B:77:TYR:O	2:B:81:ARG:HG3	2.04	0.58
2:A:186:SER:O	2:A:188:THR:N	2.36	0.58
2:A:132:LYS:HD2	2:A:282:ARG:HD2	1.85	0.58
2:A:326:ARG:NE	2:A:326:ARG:O	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:B:193:MET:CE	2:B:222:GLU:HG3	2.33	0.58
2:A:326:ARG:NH2	2:A:331:GLU:O	2.36	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:B:60:ASN:O	2:B:61:ARG:HD2	2.04	0.57
2:A:71:VAL:O	2:A:74:TYR:HB3	2.03	0.57
2:B:45:LEU:HA	2:B:94:GLN:HG3	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:304:VAL:HG12	2:A:305:SER:O	2.04	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:B:181:ARG:CD	2:B:183:LYS:HD3	2.34	0.57
2:A:225:ILE:HG22	2:A:226:SER:N	2.18	0.57
2:A:174:ILE:O	2:A:177:ILE:HB	2.05	0.56
2:A:271:LEU:HD22	2:A:271:LEU:O	2.05	0.56
2:A:122:LYS:HG3	2:A:123:GLU:N	2.20	0.56
2:B:121:ARG:HB3	2:B:121:ARG:HH11	1.69	0.56
2:A:306:ILE:N	2:A:307:PRO:CD	2.69	0.56
1:D:12:DA:OP1	2:A:81:ARG:NH2	2.37	0.56
2:A:271:LEU:HD13	2:A:272:ILE:HG13	1.88	0.56
2:A:74:TYR:O	2:A:77:TYR:HB3	2.04	0.56
2:B:23:VAL:HG22	2:B:102:SER:O	2.04	0.56
2:A:64:PHE:CZ	2:A:104:LEU:HD11	2.40	0.56
1:C:15:DG:H2''	1:C:16:DC:H5''	1.87	0.56
2:B:39:GLU:H	2:B:39:GLU:CD	2.07	0.56
2:B:132:LYS:NZ	3:B:393:HOH:O	2.34	0.56
2:B:188:THR:HG22	2:B:194:LEU:HD12	1.86	0.56
2:A:83:LEU:HD13	2:A:87:THR:HG21	1.88	0.56
2:A:71:VAL:O	2:A:74:TYR:N	2.39	0.56
2:A:213:LEU:CD1	2:A:221:VAL:HG21	2.36	0.55
2:A:83:LEU:HD23	2:A:83:LEU:N	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:B:199:ARG:O	2:B:200:THR:HG22	2.06	0.54
2:B:45:LEU:HD23	2:B:94:GLN:HG3	1.89	0.54
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:112:ALA:O	2:A:116:VAL:HG22	2.07	0.54
2:B:134:ALA:HA	2:B:283:TYR:CD2	2.43	0.54
2:A:122:LYS:CG	2:A:123:GLU:N	2.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:DC:H4'	2:A:241:ARG:HD3	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
2:A:23:VAL:HG23	2:A:27:LEU:HD21	1.89	0.54
2:B:181:ARG:HG2	3:B:439:HOH:O	2.08	0.54
1:D:22:DC:H2'	1:D:23:DT:H72	1.90	0.54
2:A:96:ASN:CG	2:A:108:SER:HB2	2.29	0.54
1:C:33:DT:H2''	1:C:34:DA:C8	2.43	0.54
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:A:125:VAL:O	2:A:125:VAL:HG12	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:67:GLU:O	2:A:70:ASP:HB2	2.08	0.53
2:A:30:MET:HG2	2:A:42:TRP:HH2	1.73	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
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:N	2:A:277:ASP:OD1	2.40	0.52
2:A:133:GLN:O	2:A:134:ALA:CB	2.57	0.52
1:C:6:DC:H2''	1:C:7:DT:O5'	2.10	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:D:17:DA:H2'	1:D:18:DT:C6	2.45	0.51
2:B:199:ARG:C	2:B:200:THR:HG22	2.31	0.51
1:C:5:DA:C2	1:C:6:DC:C2	2.99	0.51
1:D:33:DT:H2''	1:D:34:DA:N7	2.26	0.51
2:A:245:ASN:H	2:A:245:ASN:ND2	2.08	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:B:181:ARG:O	2:B:184:ASP:HB2	2.10	0.51
2:B:156:GLN:HE21	2:B:159:ARG:NH2	2.09	0.51
2:A:76:LEU:HD21	2:A:116:VAL:HG12	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:SER:HB3	3:B:402:HOH:O	2.11	0.51
1:D:5:DA:C2'	1:D:6:DC:H5'	2.40	0.51
2:A:185:ILE:HG21	2:A:193:MET:SD	2.50	0.51
2:A:282:ARG:HH11	2:A:282:ARG:HG3	1.76	0.51
2:A:126:ASP:N	2:A:126:ASP:OD1	2.44	0.51
2:B:278:ASP:OD2	2:B:279:SER:N	2.43	0.51
1:C:22:DC:H4'	2:B:118:ARG:NH2	2.25	0.51
2:A:177:ILE:O	2:A:180:ILE:CG2	2.54	0.51
2:A:130:ARG:CD	3:A:374:HOH:O	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:233:ASP:OD1	2:B:234:PRO:HD2	2.12	0.50
2:B:169:ASN:HD22	2:B:217:VAL:HG21	1.76	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:154:ARG:HH21	2:B:156:GLN:HB3	1.76	0.50
1:C:32:DT:H2''	1:C:33:DT:OP2	2.12	0.50
2:A:234:PRO:C	2:A:236:ASN:H	2.15	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:261:LEU:HA	2:A:264:ILE:HD12	1.94	0.49
2:A:232:ASP:O	2:A:234:PRO:HD3	2.12	0.49
2:A:71:VAL:O	2:A:72:ARG:C	2.50	0.49
2:A:171:LEU:HD12	2:A:171:LEU:N	2.28	0.49
3:D:39:HOH:O	2:A:156:GLN:HB2	2.12	0.49
2:A:133:GLN:O	2:A:134:ALA:HB2	2.12	0.49
2:B:137:PHE:HD1	2:B:286:TRP:CE2	2.30	0.49
2:A:225:ILE:CG2	2:A:226:SER:N	2.75	0.49
2:B:34:ARG:HB3	2:B:42:TRP:CZ2	2.48	0.49
2:B:244:LYS:C	2:B:246:GLY:H	2.15	0.49
2:A:174:ILE:O	2:A:177:ILE:N	2.45	0.49
2:B:200:THR:O	2:B:201:LYS:C	2.50	0.49
2:A:124:ASN:O	2:A:129:GLU:HB2	2.13	0.49
2:A:33:ASP:OD1	2:B:72:ARG:NH1	2.43	0.49
2:A:166:ILE:CG1	2:A:167:ALA:N	2.71	0.49
3:D:79:HOH:O	2:A:244:LYS:HB3	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:SER:OG	2:B:208:GLY:HA2	2.13	0.49
2:B:193:MET:H	2:B:218:THR:CG2	2.25	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:B:233:ASP:O	2:B:236:ASN:HB2	2.14	0.48
2:A:119:ARG:O	2:A:123:GLU:HG3	2.14	0.48
2:A:180:ILE:CG1	2:A:238:LEU:HB2	2.39	0.48
2:A:150:GLU:O	2:A:223:ARG:NH2	2.46	0.48
2:A:307:PRO:HA	2:A:310:MET:SD	2.53	0.48
2:B:183:LYS:HE3	2:B:235:ASN:HD21	1.77	0.48
2:A:281:GLN:NE2	2:A:284:LEU:HD21	2.29	0.48
2:B:306:ILE:HG22	2:B:310:MET:SD	2.53	0.48
2:B:282:ARG:NH2	3:B:474:HOH:O	2.46	0.48
2:B:51:SER:O	2:B:54:ALA:HB3	2.13	0.48
2:B:179:ARG:NH2	2:B:199:ARG:HG2	2.29	0.48
2:A:33:ASP:CG	2:B:72:ARG:NH1	2.67	0.48
2:B:219:LYS:HA	2:B:219:LYS:HE3	1.96	0.48
2:B:166:ILE:HG22	2:B:167:ALA:N	2.27	0.48
2:A:35:GLN:HB2	3:A:399:HOH:O	2.13	0.48
2:B:181:ARG:CB	2:B:183:LYS:HG2	2.44	0.48
2:A:80:ALA:C	2:A:82:GLY:N	2.64	0.48
2:B:235:ASN:O	2:B:252:ALA:CB	2.62	0.47
2:A:249:ALA:N	2:A:250:PRO:HD3	2.29	0.47
2:A:36:ALA:O	2:B:118:ARG:NH1	2.47	0.47
2:B:56:CYS:SG	2:B:63:TRP:HA	2.54	0.47
1:D:6:DC:C6	1:D:7:DT:H72	2.48	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:236:ASN:HA	2:A:251:SER:O	2.15	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: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: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:31:PHE:O	2:B:34:ARG:HG2	2.14	0.47
2:B:310:MET:O	2:B:314:GLY:N	2.45	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
1:D:20:DT:H5'	1:D:20:DT:H6	1.80	0.47
2:A:192:ARG:HD3	2:A:215:LEU:HG	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:121:ARG:CB	2:A:121:ARG:HH11	2.26	0.46
2:A:39:GLU:HG3	2:A:39:GLU:H	1.42	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:B:156:GLN:NE2	2:B:159:ARG:NH2	2.63	0.46
2:B:28:MET:O	2:B:32:ARG:HB2	2.16	0.46
1:D:5:DA:H5'	2:A:244:LYS:CB	2.45	0.46
2:A:146:ARG:O	2:A:150:GLU:CB	2.64	0.46
2:B:228:SER:OG	2:B:230:VAL:HG22	2.16	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:A:181:ARG:HD3	2:A:237:TYR:CE2	2.51	0.45
1:C:17:DA:C8	1:C:17:DA:H5''	2.51	0.45
2:A:234:PRO:C	2:A:236:ASN:N	2.69	0.45
2:B:199:ARG:C	2:B:200:THR:CG2	2.84	0.45
2:A:137:PHE:HB2	2:A:290:SER:HB3	1.98	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
2:A:271:LEU:HD13	2:A:271:LEU:O	2.16	0.45
2:A:234:PRO:C	2:A:235:ASN:CG	2.75	0.45
2:A:174:ILE:HD12	2:A:258:THR:CB	2.45	0.45
1:C:17:DA:C2	1:D:21:DG:N2	2.84	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
2:B:122:LYS:NZ	3:B:436:HOH:O	2.41	0.45
1:D:5:DA:H5''	2:A:244:LYS:HA	1.99	0.45
2:A:106:ARG:HB2	2:A:109:ASP:CG	2.37	0.45
2:A:326:ARG:HH22	2:A:331:GLU:C	2.20	0.45
2:A:326:ARG:CZ	2:A:331:GLU:HB2	2.46	0.45
2:A:92:LEU:HD11	2:A:113:VAL:CG1	2.47	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
2:A:174:ILE:HD12	2:A:258:THR:CG2	2.47	0.44
1:D:17:DA:H2'	1:D:18:DT:C5	2.53	0.44
2:A:236:ASN:HB3	2:A:237:TYR:H	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:176:GLU:HG3	2:A:179:ARG:HH11	1.82	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:170:THR:OG1	2:A:172:LEU:HG	2.16	0.44
2:A:72:ARG:HG3	2:A:116:VAL:HG11	1.99	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:A:39:GLU:O	2:A:43:LYS:HD3	2.17	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:B:304:VAL:HG12	2:B:305:SER:N	2.33	0.44
2:A:192:ARG:HD3	2:A:214:SER:O	2.17	0.44
2:A:172:LEU:HD21	2:A:211:LYS:HE3	1.99	0.44
2:A:257:SER:O	2:A:261:LEU:CD1	2.66	0.43
2:A:243:ARG:NH1	2:A:243:ARG:HG3	2.05	0.43
2:A:132:LYS:CD	2:A:282:ARG:HD2	2.48	0.43
2:A:176:GLU:O	2:A:180:ILE:HG22	2.18	0.43
2:B:113:VAL:O	2:B:116:VAL:HG12	2.19	0.43
1:D:11:DT:H2"	1:D:12:DA:OP2	2.17	0.43
2:B:52:TRP:CZ2	2:B:66:ALA:HB2	2.53	0.43
1:D:22:DC:OP2	2:B:100:ARG:NH2	2.51	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:B:67:GLU:CD	2:B:68:PRO:HD2	2.39	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: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:118:ARG:O	2:B:122:LYS:HG3	2.19	0.43
2:B:70:ASP:HA	2:B:73:ASP:OD2	2.19	0.43
2:A:187:ARG:HG3	2:A:191:GLY:O	2.19	0.43
2:B:179:ARG:NH2	3:B:384:HOH:O	2.45	0.43
2:B:92:LEU:HD12	2:B:92:LEU:O	2.19	0.43
2:A:245:ASN:N	2:A:245:ASN:ND2	2.62	0.43
2:A:304:VAL:CG1	2:A:308:GLU:HB2	2.49	0.43
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
1:C:22:DC:H5"	2:A:37:PHE:CE2	2.54	0.43
2:B:225:ILE:HG22	2:B:226:SER:N	2.33	0.43
2:A:189:ASP:C	2:A:191:GLY:H	2.23	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:177:ILE:HA	2:B:180:ILE:HD12	2.01	0.42
2:A:330:SER:O	2:A:332:THR:N	2.49	0.42
2:A:259:ARG:CG	2:A:259:ARG:NH1	2.74	0.42
2:B:23:VAL:HG12	2:B:24:ARG:N	2.32	0.42
2:A:179:ARG:NH2	3:A:383:HOH:O	2.52	0.42
1:D:24:DA:H5''	2:B:201:LYS:CB	2.39	0.42
2:B:213:LEU:CB	2:B:218:THR:HG22	2.43	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:A:37:PHE:CZ	2:A:97:MET:HE2	2.54	0.42
2:A:259:ARG:CG	2:A:259:ARG:HH11	2.15	0.42
2:B:85:VAL:HG23	2:B:129:GLU:OE2	2.18	0.42
2:A:174:ILE:O	2:A:175:ALA:C	2.58	0.42
1:D:22:DC:H2'	1:D:23:DT:C7	2.49	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:B:159:ARG:O	2:B:162:ALA:N	2.52	0.42
2:A:104:LEU:HG	2:A:104:LEU:H	1.57	0.42
2:A:97:MET:O	2:A:101:ARG:HG2	2.20	0.42
2:B:122:LYS:HE3	2:B:122:LYS:HB3	1.86	0.42
2:B:197:ILE:CD1	2:B:211:LYS:HG3	2.49	0.42
2:B:192:ARG:NH1	2:B:215:LEU:HG	2.34	0.42
1:D:20:DT:C4	1:D:21:DG:C6	3.08	0.42
2:A:182:VAL:CG2	2:A:234:PRO:HA	2.49	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:243:ARG:NH1	2:A:243:ARG:CG	2.68	0.42
2:B:185:ILE:HD11	2:B:238:LEU:HD13	2.01	0.42
2:A:306:ILE:H	2:A:307:PRO:HD3	1.85	0.42
2:A:326:ARG:NH2	2:A:331:GLU:C	2.73	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:B:181:ARG:HB2	2:B:183:LYS:HG2	2.02	0.41
2:A:243:ARG:CB	2:A:245:ASN:ND2	2.83	0.41
1:D:24:DA:H2''	1:D:25:DT:C7	2.49	0.41
1:D:3:DT:H3'	3:D:84:HOH:O	2.19	0.41
2:B:235:ASN:O	2:B:252:ALA:HB1	2.19	0.41
2:A:185:ILE:CG2	2:A:193:MET:SD	3.07	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:193:MET:H	2:A:193:MET:HG2	1.59	0.41
2:B:271:LEU:HD23	2:B:272:ILE:CD1	2.51	0.41
2:A:158:ILE:O	2:A:159:ARG:C	2.57	0.41
2:B:171:LEU:O	2:B:292:ARG:NH1	2.53	0.41
1:D:14:DA:H2'	3:D:46:HOH:O	2.21	0.41
1:C:6:DC:H2''	1:C:7:DT:C5'	2.50	0.41
1:C:14:DA:N7	2:B:86:LYS:HD3	2.36	0.41
2:A:80:ALA:C	2:A:82:GLY:H	2.23	0.41
2:A:22:GLU:OE2	3:A:409:HOH:O	2.21	0.41
2:A:231:ALA:O	2:A:232:ASP:O	2.39	0.41
2:B:29:ASP:O	2:B:32:ARG:HB3	2.20	0.41
1:C:14:DA:C8	2:B:86:LYS:HD3	2.56	0.41
2:B:308:GLU:O	2:B:311:GLN:HB3	2.20	0.41
2:B:111:ASN:O	2:B:115:LEU:HD12	2.20	0.41
2:B:181:ARG:HB3	2:B:183:LYS:HG2	2.02	0.41
2:B:40:HIS:HA	2:B:43:LYS:HB2	2.03	0.40
2:B:130:ARG:HD2	2:B:130:ARG:N	2.36	0.40
2:A:165:GLY:O	2:A:169:ASN:HB2	2.20	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:138:GLU:N	2:B:141:ASP:OD2	2.53	0.40
2:A:271:LEU:C	2:A:271:LEU:CD1	2.88	0.40
2:B:128:GLY:O	2:B:130:ARG:HG3	2.21	0.40
1:D:6:DC:H2''	1:D:7:DT:H73	1.97	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:HB3	2:A:270:ARG:CZ	2.50	0.40
2:A:245:ASN:ND2	2:A:247:VAL:H	2.20	0.40
2:A:326:ARG:HE	2:A:329:ASP:HB2	1.87	0.40
1:C:23:DT:H71	2:A:41:THR:HG23	2.04	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

5.3.1 Protein backbone

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%)	1	1
2	B	294/343 (86%)	261 (89%)	28 (10%)	5 (2%)	11	29
All	All	585/686 (85%)	477 (82%)	77 (13%)	31 (5%)	2	4

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	163 (66%)	84 (34%)	0	0
2	B	245/287 (85%)	191 (78%)	54 (22%)	1	3
All	All	492/574 (86%)	354 (72%)	138 (28%)	0	1

All (138) 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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	122	LYS
2	A	129	GLU
2	A	130	ARG
2	A	132	LYS
2	A	139	ARG
2	A	140	THR
2	A	147	SER
2	A	151	ASN
2	A	155	CYS
2	A	156	GLN
2	A	157	ASP
2	A	160	ASN
2	A	161	LEU
2	A	166	ILE
2	A	173	ARG
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	192	ARG
2	A	193	MET
2	A	211	LYS
2	A	214	SER
2	A	215	LEU
2	A	219	LYS
2	A	224	TRP
2	A	225	ILE
2	A	235	ASN
2	A	238	LEU
2	A	241	ARG
2	A	243	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	330	SER
2	A	332	THR
2	A	335	MET
2	A	339	LEU
2	B	20	SER
2	B	24	ARG
2	B	27	LEU
2	B	28	MET
2	B	34	ARG
2	B	35	GLN
2	B	38	SER
2	B	43	LYS
2	B	45	LEU
2	B	58	LEU
2	B	60	ASN
2	B	62	LYS
2	B	73	ASP
2	B	77	TYR
2	B	83	LEU
2	B	86	LYS
2	B	87	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	90	GLN
2	B	94	GLN
2	B	95	LEU
2	B	96	ASN
2	B	106	ARG
2	B	110	SER
2	B	114	SER
2	B	121	ARG
2	B	125	VAL
2	B	130	ARG
2	B	132	LYS
2	B	139	ARG
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	204	VAL
2	B	219	LYS
2	B	226	SER
2	B	245	ASN
2	B	257	SER
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	298	ASP
2	B	299	MET
2	B	305	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	59	ASN
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	59	ASN
2	B	60	ASN
2	B	79	GLN
2	B	90	GLN
2	B	94	GLN
2	B	151	ASN
2	B	169	ASN
2	B	245	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.