Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:39 AM GMT

PDB ID	:	2NQP
Title	:	Crystal structure of pseudoudirinde synthase TruA in complex with leucyl tRNA
Authors	:	Hur, S.; Stroud, R.M.
Deposited on	:	2006-10-31
Resolution	:	3.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

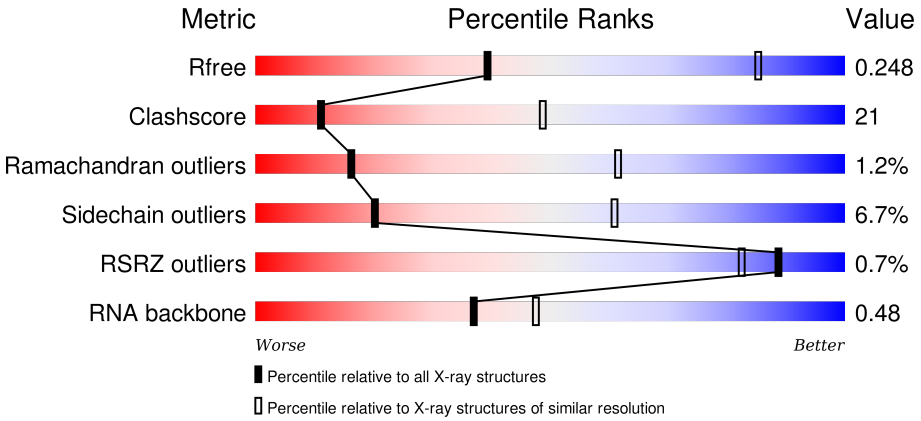
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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 <=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	F	87	7%, 23%, 44%, 13%, ·, 18%
2	A	270	53%, 43%, · ·
2	B	270	58%, 37%, · ·
2	C	270	57%, 39%, · ·

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Mol	Chain	Length	Quality of chain
2	D	270	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9765 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 RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	71	Total	C	N	O	P	21	0	0
			1441	636	256	480	69			

- Molecule 2 is a protein called tRNA pseudouridine synthase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	264	Total	C	N	O	S	0	0	0
			2088	1327	379	374	8			
2	B	264	Total	C	N	O	S	0	0	0
			2083	1325	377	373	8			
2	C	264	Total	C	N	O	S	0	0	0
			2057	1306	373	370	8			
2	D	263	Total	C	N	O	S	18	0	0
			2090	1328	381	373	8			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

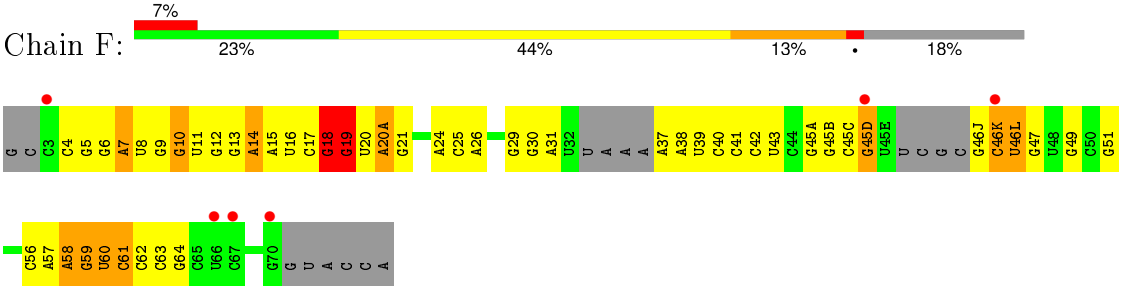
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	K	0	0
			1	1		
3	F	5	Total	K	0	0
			5	5		

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.

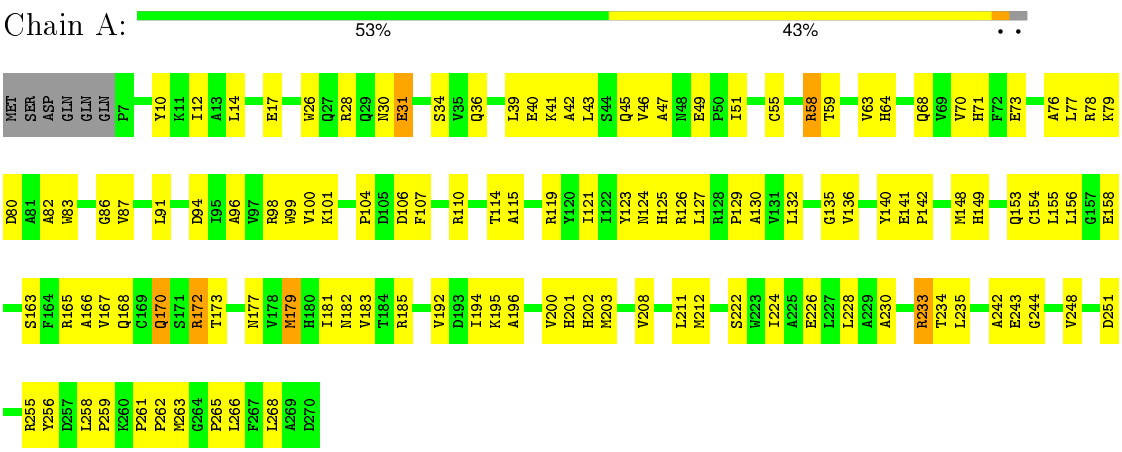
- Molecule 1: transfer RNA

Chain F:



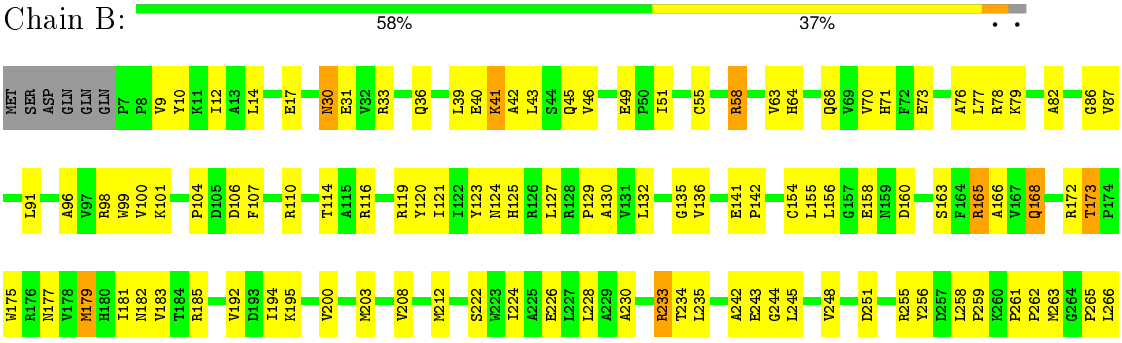
- Molecule 2: tRNA pseudouridine synthase A

Chain A:



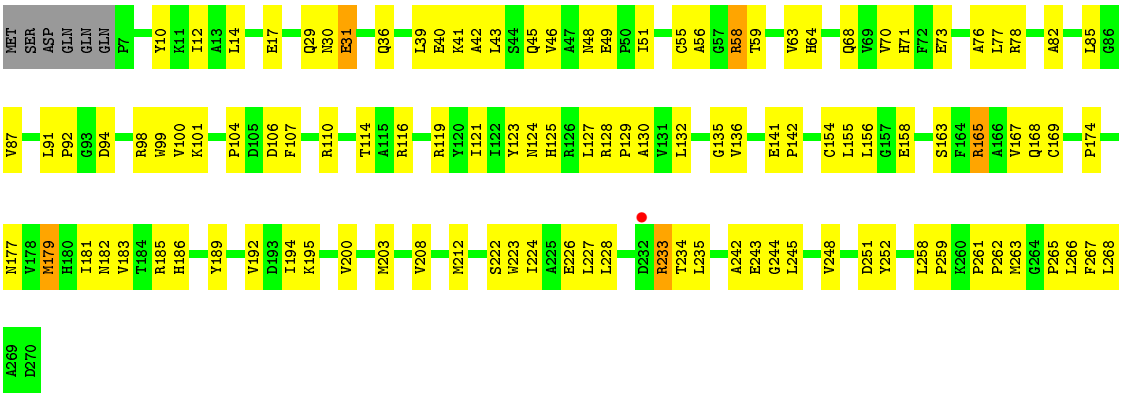
- Molecule 2: tRNA pseudouridine synthase A

Chain B:



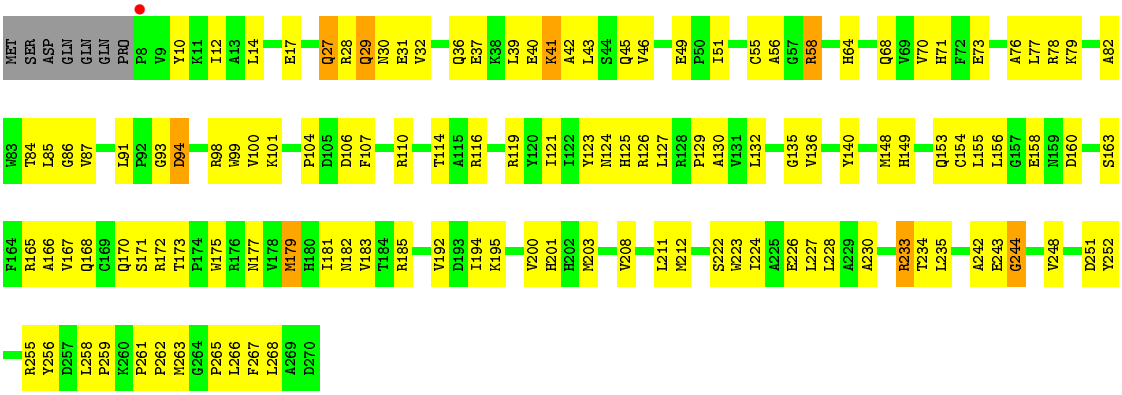
• Molecule 2: tRNA pseudouridine synthase A

Chain C:



• Molecule 2: tRNA pseudouridine synthase A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.28Å 128.59Å 159.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 77.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.50) 92.4 (77.07-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.279 0.224 , 0.248	Depositor DCC
R_{free} test set	2528 reflections (11.73%)	DCC
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 30274 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9765	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	F	0.63	2/1604 (0.1%)	0.88	5/2498 (0.2%)
2	A	0.52	0/2142	0.65	0/2915
2	B	0.51	0/2139	0.65	0/2912
2	C	0.47	0/2112	0.64	0/2881
2	D	0.49	0/2145	0.62	0/2917
All	All	0.52	2/10142 (0.0%)	0.69	5/14123 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	46(L)	U	C2-N3	-5.32	1.34	1.37
1	F	18	G	O3'-P	-5.20	1.54	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	19	G	O4'-C1'-N9	-8.26	101.59	108.20
1	F	46(L)	U	OP1-P-OP2	-6.44	109.94	119.60
1	F	19	G	OP1-P-OP2	-6.44	109.94	119.60
1	F	46(K)	C	P-O3'-C3'	-5.32	113.32	119.70
1	F	46(L)	U	C6-N1-C2	5.11	124.07	121.00

There are no chirality outliers.

There are no planarity outliers.

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	F	1441	0	722	44	0
2	A	2088	0	2039	93	0
2	B	2083	0	2039	85	0
2	C	2057	0	1982	86	0
2	D	2090	0	2059	99	0
3	C	1	0	0	0	0
3	F	5	0	0	0	0
All	All	9765	0	8841	383	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 21.

All (383) 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)
2:A:130:ALA:HB3	2:B:17:GLU:HG2	1.46	0.95
2:A:17:GLU:HG2	2:B:130:ALA:HB3	1.51	0.92
2:C:130:ALA:HB1	2:D:94:ASP:O	1.70	0.88
1:F:58:A:H4'	1:F:59:G:OP1	1.70	0.88
2:A:41:LYS:CA	2:A:42:ALA:N	2.41	0.83
2:D:165:ARG:HG2	2:D:166:ALA:H	1.43	0.82
2:D:27:GLN:HE22	2:D:58:ARG:HD3	1.43	0.81
2:A:132:LEU:HD13	2:B:132:LEU:HD13	1.63	0.81
2:B:14:LEU:HD11	2:B:43:LEU:HD21	1.67	0.77
1:F:16:U:O4	1:F:19:G:H8	1.67	0.77
1:F:25:C:OP1	2:D:167:VAL:HG22	1.85	0.76
2:C:30:ASN:N	2:C:31:GLU:OE2	2.19	0.76
2:D:27:GLN:HA	2:D:27:GLN:HE21	1.50	0.76
2:A:155:LEU:HD23	2:A:228:LEU:HD22	1.68	0.76
2:B:222:SER:O	2:B:226:GLU:HG3	1.86	0.75
1:F:45(A):G:H1	1:F:46(L):U:H3	1.35	0.75
2:A:222:SER:O	2:A:226:GLU:HG3	1.86	0.74
2:C:222:SER:O	2:C:226:GLU:HG3	1.88	0.73
2:A:126:ARG:HG3	2:A:140:TYR:CE1	2.23	0.73
1:F:60:U:H5"	1:F:61:C:OP2	1.86	0.73
2:D:29:GLN:HB3	2:D:32:VAL:HG22	1.70	0.73
2:D:27:GLN:NE2	2:D:58:ARG:HD3	2.03	0.73
2:A:233:ARG:O	2:A:233:ARG:HD3	1.88	0.73
2:D:222:SER:O	2:D:226:GLU:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:C:H2'	1:F:41:C:C6	2.25	0.71
2:A:41:LYS:CA	2:A:41:LYS:O	2.39	0.71
1:F:16:U:H1'	2:D:140:TYR:CZ	2.25	0.71
2:D:126:ARG:HG3	2:D:140:TYR:CE1	2.25	0.71
2:A:14:LEU:HD11	2:A:43:LEU:HD21	1.71	0.71
2:C:14:LEU:HD11	2:C:43:LEU:HD21	1.71	0.70
2:A:41:LYS:O	2:A:42:ALA:N	2.24	0.70
2:D:14:LEU:HD11	2:D:43:LEU:HD21	1.71	0.70
2:D:233:ARG:O	2:D:233:ARG:HD3	1.91	0.70
2:D:155:LEU:HD23	2:D:228:LEU:HD22	1.72	0.70
1:F:29:G:H2'	1:F:30:G:C8	2.27	0.70
2:A:181:ILE:HD12	2:A:194:ILE:HD12	1.73	0.69
2:C:132:LEU:HD13	2:D:132:LEU:HD13	1.73	0.69
2:C:233:ARG:O	2:C:233:ARG:HD3	1.93	0.68
1:F:46(J):G:H2'	1:F:46(K):C:C6	2.28	0.68
2:C:155:LEU:HD23	2:C:228:LEU:HD22	1.75	0.68
2:B:155:LEU:HD23	2:B:228:LEU:HD22	1.75	0.68
2:B:233:ARG:O	2:B:233:ARG:HD3	1.93	0.68
2:B:173:THR:O	2:B:173:THR:HG23	1.93	0.68
2:C:181:ILE:HD12	2:C:194:ILE:HD12	1.77	0.67
2:D:39:LEU:HA	2:D:91:LEU:HD21	1.77	0.67
2:B:39:LEU:HA	2:B:91:LEU:HD21	1.76	0.67
2:A:39:LEU:HA	2:A:91:LEU:HD21	1.75	0.66
2:D:166:ALA:HB3	2:D:201:HIS:HB3	1.76	0.66
2:D:76:ALA:HB1	2:D:78:ARG:HH12	1.60	0.66
2:C:248:VAL:HB	2:C:263:MET:HB2	1.77	0.66
2:C:132:LEU:HD23	2:C:136:VAL:HG13	1.79	0.65
2:D:248:VAL:HB	2:D:263:MET:HB2	1.78	0.65
2:A:248:VAL:HB	2:A:263:MET:HB2	1.79	0.64
2:A:124:ASN:ND2	2:A:185:ARG:HH22	1.96	0.64
2:B:181:ILE:HD12	2:B:194:ILE:HD12	1.79	0.64
2:C:39:LEU:HA	2:C:91:LEU:HD21	1.78	0.64
2:D:76:ALA:HB1	2:D:78:ARG:NH1	2.12	0.64
2:C:76:ALA:HB1	2:C:78:ARG:HH12	1.63	0.63
2:B:248:VAL:HB	2:B:263:MET:HB2	1.81	0.63
1:F:25:C:H5"	2:D:167:VAL:HG11	1.79	0.63
2:A:36:GLN:O	2:A:40:GLU:HG3	1.99	0.63
2:B:36:GLN:O	2:B:40:GLU:HG3	1.99	0.63
2:C:76:ALA:HB1	2:C:78:ARG:NH1	2.13	0.63
2:D:181:ILE:HD12	2:D:194:ILE:HD12	1.79	0.63
2:C:36:GLN:O	2:C:40:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASN:ND2	2:C:185:ARG:HH22	1.97	0.62
2:C:123:TYR:HD2	2:C:129:PRO:HD3	1.65	0.62
2:A:99:TRP:CD2	2:A:259:PRO:HG2	2.35	0.61
2:D:124:ASN:ND2	2:D:185:ARG:HH22	1.98	0.61
1:F:46(J):G:H2'	1:F:46(K):C:H6	1.65	0.61
2:C:17:GLU:HG2	2:D:130:ALA:HB3	1.81	0.61
2:B:160:ASP:HB2	2:B:175:TRP:CZ2	2.35	0.61
2:B:132:LEU:HD23	2:B:136:VAL:HG13	1.83	0.61
2:D:132:LEU:HD23	2:D:136:VAL:HG13	1.83	0.61
1:F:18:G:C5	1:F:57:A:N6	2.69	0.61
2:A:55:CYS:HB2	2:A:68:GLN:OE1	2.02	0.60
2:B:123:TYR:HD2	2:B:129:PRO:HD3	1.67	0.60
2:B:125:HIS:CD2	2:B:127:LEU:H	2.20	0.60
2:A:266:LEU:HD13	2:B:266:LEU:HD13	1.83	0.60
2:D:125:HIS:CD2	2:D:127:LEU:H	2.20	0.59
2:A:76:ALA:HB1	2:A:78:ARG:NH1	2.16	0.59
2:A:125:HIS:CD2	2:A:127:LEU:H	2.20	0.59
2:D:29:GLN:CB	2:D:32:VAL:HG22	2.32	0.59
2:B:30:ASN:ND2	2:B:30:ASN:H	1.99	0.59
2:B:82:ALA:O	2:B:86:GLY:HA3	2.03	0.59
2:B:104:PRO:HB2	2:B:106:ASP:OD2	2.03	0.59
1:F:63:C:H2'	1:F:64:G:C8	2.37	0.59
2:C:266:LEU:HD13	2:D:266:LEU:HD13	1.85	0.59
2:D:36:GLN:O	2:D:40:GLU:HG3	2.03	0.59
2:A:132:LEU:HD23	2:A:136:VAL:HG13	1.84	0.58
2:A:76:ALA:HB1	2:A:78:ARG:HH12	1.68	0.58
2:D:104:PRO:HB2	2:D:106:ASP:OD2	2.03	0.58
2:D:99:TRP:CD2	2:D:259:PRO:HG2	2.38	0.58
1:F:42:C:O2'	1:F:43:U:H5'	2.03	0.58
2:A:165:ARG:HD2	2:A:200:VAL:HG11	1.85	0.58
2:A:104:PRO:HB2	2:A:106:ASP:OD2	2.03	0.57
2:C:55:CYS:HB2	2:C:68:GLN:OE1	2.04	0.57
2:B:124:ASN:ND2	2:B:185:ARG:HH22	2.02	0.57
2:C:125:HIS:CD2	2:C:127:LEU:H	2.22	0.57
2:D:27:GLN:HE22	2:D:58:ARG:CD	2.16	0.57
2:C:123:TYR:CD2	2:C:129:PRO:HD3	2.39	0.57
2:C:98:ARG:HH21	2:C:261:PRO:HB2	1.69	0.57
2:A:55:CYS:HA	2:A:70:VAL:HG12	1.87	0.56
2:B:98:ARG:HH21	2:B:261:PRO:HB2	1.70	0.56
1:F:10:G:H2'	1:F:11:U:C6	2.40	0.56
2:C:104:PRO:HB2	2:C:106:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:166:ALA:HB3	2:A:201:HIS:HB3	1.88	0.56
2:B:123:TYR:CD2	2:B:129:PRO:HD3	2.40	0.56
2:C:167:VAL:C	2:C:169:CYS:H	2.09	0.56
1:F:4:C:H2'	1:F:5:G:C8	2.41	0.56
2:B:76:ALA:HB1	2:B:78:ARG:NH1	2.21	0.56
2:C:29:GLN:C	2:C:31:GLU:OE2	2.43	0.55
2:D:123:TYR:HD2	2:D:129:PRO:HD3	1.71	0.55
2:C:99:TRP:CD2	2:C:259:PRO:HG2	2.41	0.55
2:A:124:ASN:HD22	2:A:185:ARG:HH22	1.53	0.55
2:A:10:TYR:O	2:A:73:GLU:HA	2.07	0.55
2:D:233:ARG:C	2:D:235:LEU:H	2.10	0.55
2:B:76:ALA:HB1	2:B:78:ARG:HH12	1.71	0.55
2:B:10:TYR:O	2:B:73:GLU:HA	2.06	0.55
2:B:99:TRP:CD2	2:B:259:PRO:HG2	2.41	0.55
2:B:200:VAL:O	2:B:203:MET:HB2	2.07	0.55
2:A:123:TYR:HD2	2:A:129:PRO:HD3	1.71	0.55
2:B:78:ARG:HB3	2:B:82:ALA:CB	2.37	0.54
2:C:127:LEU:HD11	2:D:84:THR:HB	1.89	0.54
2:C:124:ASN:HD22	2:C:185:ARG:HH22	1.55	0.54
2:C:55:CYS:HA	2:C:70:VAL:HG12	1.90	0.54
2:B:49:GLU:O	2:B:51:ILE:HG12	2.08	0.54
2:D:55:CYS:HB2	2:D:68:GLN:OE1	2.06	0.54
2:D:10:TYR:O	2:D:73:GLU:HA	2.07	0.54
2:C:78:ARG:HB3	2:C:82:ALA:CB	2.37	0.54
2:D:98:ARG:HH21	2:D:261:PRO:HB2	1.72	0.54
2:B:55:CYS:HB2	2:B:68:GLN:OE1	2.08	0.54
2:C:200:VAL:O	2:C:203:MET:HB2	2.07	0.54
2:A:121:ILE:HD11	2:A:268:LEU:HD11	1.89	0.54
2:B:168:GLN:O	2:B:168:GLN:HG2	2.08	0.54
2:C:165:ARG:CZ	2:C:174:PRO:HB3	2.38	0.54
1:F:39:U:H2'	1:F:40:C:O4'	2.07	0.54
2:B:55:CYS:HA	2:B:70:VAL:HG12	1.90	0.54
2:B:17:GLU:HB2	2:B:98:ARG:HD2	1.91	0.53
2:B:233:ARG:C	2:B:235:LEU:H	2.12	0.53
2:A:42:ALA:HA	2:A:45:GLN:HE21	1.73	0.53
2:C:10:TYR:O	2:C:73:GLU:HA	2.09	0.53
2:D:123:TYR:CD2	2:D:129:PRO:HD3	2.44	0.53
1:F:45(A):G:O2'	1:F:45(B):G:H5'	2.09	0.53
2:B:121:ILE:HD11	2:B:268:LEU:HD11	1.91	0.53
2:D:55:CYS:HA	2:D:70:VAL:HG12	1.90	0.53
2:A:181:ILE:C	2:A:182:ASN:HD22	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:ILE:C	2:A:182:ASN:ND2	2.62	0.52
2:A:78:ARG:HB3	2:A:82:ALA:CB	2.40	0.52
1:F:19:G:N1	2:C:82:ALA:HA	2.24	0.52
2:C:167:VAL:O	2:C:169:CYS:N	2.39	0.52
2:D:27:GLN:CA	2:D:27:GLN:HE21	2.21	0.52
2:D:165:ARG:HG2	2:D:166:ALA:N	2.19	0.52
2:A:123:TYR:CD2	2:A:129:PRO:HD3	2.44	0.52
2:A:43:LEU:HD23	2:A:87:VAL:HG21	1.91	0.52
2:D:78:ARG:HB3	2:D:82:ALA:CB	2.40	0.52
2:B:78:ARG:HB3	2:B:82:ALA:HB3	1.91	0.51
2:D:17:GLU:HB2	2:D:98:ARG:HD2	1.93	0.51
2:D:49:GLU:O	2:D:51:ILE:HG12	2.10	0.51
1:F:30:G:H2'	1:F:31:A:H8	1.76	0.51
2:A:78:ARG:HB3	2:A:82:ALA:HB3	1.92	0.51
2:A:17:GLU:HB2	2:A:98:ARG:HD2	1.93	0.51
2:D:124:ASN:HD22	2:D:185:ARG:HH22	1.57	0.51
2:B:30:ASN:N	2:B:30:ASN:ND2	2.56	0.51
2:D:121:ILE:HD11	2:D:268:LEU:HD11	1.92	0.51
2:B:43:LEU:HD23	2:B:87:VAL:HG21	1.93	0.51
2:D:183:VAL:HG22	2:D:192:VAL:HG22	1.92	0.51
2:C:49:GLU:O	2:C:51:ILE:HG12	2.11	0.51
2:C:154:CYS:SG	2:C:224:ILE:HG22	2.50	0.51
2:C:121:ILE:HD11	2:C:268:LEU:HD11	1.92	0.51
2:A:154:CYS:SG	2:A:224:ILE:HG22	2.51	0.51
2:A:96:ALA:HB3	2:B:130:ALA:HB2	1.93	0.51
2:A:42:ALA:HA	2:A:45:GLN:NE2	2.26	0.51
2:A:233:ARG:C	2:A:233:ARG:HD3	2.31	0.51
2:A:208:VAL:O	2:A:212:MET:HG3	2.10	0.51
2:C:42:ALA:HA	2:C:45:GLN:HE21	1.76	0.51
2:D:43:LEU:HD23	2:D:87:VAL:HG21	1.92	0.51
2:B:181:ILE:C	2:B:182:ASN:HD22	2.14	0.51
2:C:242:ALA:O	2:C:244:GLY:N	2.44	0.51
2:B:154:CYS:SG	2:B:224:ILE:HG22	2.50	0.51
2:B:158:GLU:HG2	2:B:177:ASN:HB2	1.92	0.51
2:A:233:ARG:C	2:A:235:LEU:H	2.13	0.51
2:C:181:ILE:C	2:C:182:ASN:HD22	2.14	0.51
2:A:58:ARG:NH2	2:A:110:ARG:HH12	2.07	0.51
2:A:98:ARG:HH21	2:A:261:PRO:HB2	1.74	0.51
2:D:28:ARG:CZ	2:D:37:GLU:HG3	2.41	0.51
2:C:107:PHE:CZ	2:C:258:LEU:HD11	2.46	0.50
2:B:183:VAL:HG22	2:B:192:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:C:H6	1:F:62:C:O5'	1.94	0.50
1:F:30:G:H8	1:F:30:G:O5'	1.94	0.50
2:C:132:LEU:HD23	2:C:136:VAL:CG1	2.42	0.50
2:D:173:THR:O	2:D:173:THR:HG23	2.12	0.50
2:C:127:LEU:HD23	2:D:85:LEU:HD23	1.93	0.50
2:C:58:ARG:NH2	2:C:110:ARG:HH12	2.09	0.50
2:D:200:VAL:O	2:D:203:MET:HB2	2.11	0.50
2:C:78:ARG:HB3	2:C:82:ALA:HB3	1.93	0.50
2:C:267:PHE:HB2	2:D:267:PHE:HB2	1.94	0.50
2:C:183:VAL:HG22	2:C:192:VAL:HG22	1.93	0.50
2:C:233:ARG:C	2:C:235:LEU:H	2.13	0.50
2:B:181:ILE:C	2:B:182:ASN:ND2	2.65	0.50
2:C:17:GLU:HB2	2:C:98:ARG:HD2	1.94	0.50
2:B:58:ARG:NH2	2:B:110:ARG:HH12	2.09	0.50
2:C:123:TYR:CD2	2:C:129:PRO:HB3	2.46	0.49
2:A:49:GLU:O	2:A:51:ILE:HG12	2.12	0.49
2:C:208:VAL:O	2:C:212:MET:HG3	2.11	0.49
2:B:208:VAL:O	2:B:212:MET:HG3	2.13	0.49
2:A:183:VAL:HG22	2:A:192:VAL:HG22	1.93	0.49
2:D:107:PHE:CZ	2:D:258:LEU:HD11	2.48	0.49
2:D:27:GLN:NE2	2:D:58:ARG:CD	2.72	0.49
2:B:123:TYR:CD2	2:B:129:PRO:HB3	2.47	0.49
2:D:181:ILE:C	2:D:182:ASN:HD22	2.16	0.49
2:B:165:ARG:HG3	2:B:200:VAL:HB	1.95	0.49
2:D:233:ARG:C	2:D:233:ARG:HD3	2.33	0.49
2:C:181:ILE:C	2:C:182:ASN:ND2	2.66	0.49
2:A:123:TYR:CD2	2:A:129:PRO:HB3	2.48	0.49
2:A:265:PRO:HD2	2:A:268:LEU:HD12	1.95	0.49
2:D:208:VAL:O	2:D:212:MET:HG3	2.13	0.49
2:A:127:LEU:HD12	2:B:98:ARG:O	2.13	0.48
2:D:58:ARG:NH2	2:D:110:ARG:HH12	2.10	0.48
2:D:78:ARG:HB3	2:D:82:ALA:HB3	1.95	0.48
2:B:41:LYS:O	2:B:45:GLN:HG3	2.12	0.48
1:F:37:A:H2'	1:F:38:A:C8	2.48	0.48
2:D:242:ALA:O	2:D:244:GLY:N	2.46	0.48
2:D:132:LEU:HD23	2:D:136:VAL:CG1	2.43	0.48
2:A:166:ALA:HB2	2:A:202:HIS:HB2	1.94	0.48
2:B:124:ASN:HD22	2:B:185:ARG:HH22	1.60	0.48
2:D:181:ILE:C	2:D:182:ASN:ND2	2.66	0.48
2:A:158:GLU:HG2	2:A:177:ASN:HB2	1.95	0.48
1:F:42:C:H2'	1:F:43:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:PRO:HB2	2:C:262:PRO:HD2	1.96	0.48
2:C:174:PRO:HA	2:C:200:VAL:HG11	1.94	0.48
2:A:261:PRO:HB2	2:A:262:PRO:HD2	1.94	0.48
2:D:265:PRO:HD2	2:D:268:LEU:HD12	1.95	0.48
2:B:233:ARG:HD3	2:B:233:ARG:C	2.33	0.48
2:D:154:CYS:SG	2:D:224:ILE:HG22	2.54	0.48
2:D:158:GLU:HG2	2:D:177:ASN:HB2	1.96	0.48
2:C:119:ARG:HD2	2:C:248:VAL:HG11	1.95	0.47
1:F:29:G:N2	1:F:42:C:C2	2.82	0.47
2:D:123:TYR:CD2	2:D:129:PRO:HB3	2.49	0.47
2:B:58:ARG:HH21	2:B:110:ARG:HH12	1.61	0.47
1:F:18:G:C5	1:F:57:A:C6	3.02	0.47
2:B:265:PRO:HD2	2:B:268:LEU:HD12	1.95	0.47
2:B:242:ALA:O	2:B:244:GLY:N	2.47	0.47
2:C:233:ARG:C	2:C:233:ARG:HD3	2.33	0.47
2:C:12:ILE:O	2:C:71:HIS:HA	2.15	0.47
2:A:130:ALA:CB	2:B:17:GLU:HG2	2.32	0.47
1:F:8:U:H2'	1:F:21:G:N2	2.29	0.47
2:A:107:PHE:CZ	2:A:258:LEU:HD11	2.50	0.47
2:A:115:ALA:HB1	2:A:196:ALA:O	2.15	0.47
2:C:42:ALA:HA	2:C:45:GLN:NE2	2.30	0.47
2:A:64:HIS:CE1	2:A:135:GLY:HA2	2.50	0.47
2:A:82:ALA:O	2:A:86:GLY:HA3	2.15	0.47
2:D:119:ARG:HD2	2:D:248:VAL:HG11	1.96	0.46
2:D:261:PRO:HB2	2:D:262:PRO:HD2	1.97	0.46
2:D:58:ARG:HH21	2:D:110:ARG:HH12	1.62	0.46
2:B:119:ARG:HD2	2:B:248:VAL:HG11	1.96	0.46
2:B:42:ALA:HA	2:B:45:GLN:NE2	2.31	0.46
2:C:64:HIS:CE1	2:C:135:GLY:HA2	2.51	0.46
2:C:265:PRO:HD2	2:C:268:LEU:HD12	1.96	0.46
2:C:158:GLU:HG2	2:C:177:ASN:HB2	1.98	0.46
2:D:179:MET:N	2:D:195:LYS:O	2.47	0.46
2:B:166:ALA:HB1	2:B:168:GLN:OE1	2.16	0.46
2:A:58:ARG:HH21	2:A:110:ARG:HH12	1.63	0.46
2:B:42:ALA:HA	2:B:45:GLN:HE21	1.79	0.46
2:A:242:ALA:O	2:A:244:GLY:N	2.49	0.46
2:A:200:VAL:O	2:A:203:MET:HB2	2.16	0.46
2:B:64:HIS:CE1	2:B:135:GLY:HA2	2.50	0.46
2:B:30:ASN:HD22	2:B:30:ASN:N	2.14	0.46
2:C:41:LYS:O	2:C:45:GLN:HG3	2.14	0.46
1:F:13:G:H2'	1:F:14:A:H5"	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:ILE:O	2:D:71:HIS:HA	2.16	0.46
2:C:43:LEU:HD23	2:C:87:VAL:HG21	1.97	0.45
1:F:56:C:O4'	2:C:48:ASN:HB2	2.16	0.45
2:B:107:PHE:CZ	2:B:258:LEU:HD11	2.50	0.45
2:C:100:VAL:HG22	2:C:101:LYS:N	2.31	0.45
2:C:58:ARG:HH21	2:C:110:ARG:HH12	1.64	0.45
2:B:64:HIS:HE1	2:B:135:GLY:HA2	1.82	0.45
1:F:58:A:O2'	1:F:59:G:O5'	2.34	0.45
2:D:230:ALA:HB1	2:D:235:LEU:HD12	1.97	0.45
1:F:45(C):C:H5'	1:F:45(D):G:OP2	2.17	0.45
2:A:230:ALA:HB1	2:A:235:LEU:HD12	1.99	0.45
2:C:94:ASP:O	2:D:130:ALA:HB1	2.17	0.45
2:D:41:LYS:O	2:D:45:GLN:HG3	2.17	0.45
1:F:29:G:H2'	1:F:30:G:H8	1.81	0.45
2:D:42:ALA:HA	2:D:45:GLN:HE21	1.82	0.45
2:A:179:MET:N	2:A:195:LYS:O	2.46	0.44
2:D:148:MET:HE3	2:D:211:LEU:O	2.17	0.44
2:A:28:ARG:HA	2:A:34:SER:OG	2.17	0.44
2:A:149:HIS:CE1	2:A:153:GLN:NE2	2.85	0.44
2:A:64:HIS:HE1	2:A:135:GLY:HA2	1.83	0.44
2:B:12:ILE:O	2:B:71:HIS:HA	2.17	0.44
2:A:30:ASN:O	2:A:31:GLU:CB	2.64	0.44
2:D:160:ASP:HB2	2:D:175:TRP:CZ2	2.51	0.44
2:A:43:LEU:HD23	2:A:87:VAL:CG2	2.47	0.44
2:C:46:VAL:HG12	2:C:78:ARG:HG3	1.99	0.44
2:B:168:GLN:N	2:B:168:GLN:OE1	2.44	0.44
1:F:25:C:H2'	1:F:26:A:O5'	2.18	0.43
2:A:126:ARG:HG3	2:A:140:TYR:CZ	2.53	0.43
2:C:141:GLU:HA	2:C:142:PRO:HD3	1.80	0.43
1:F:8:U:N3	1:F:13:G:C6	2.86	0.43
2:D:82:ALA:O	2:D:86:GLY:HA3	2.17	0.43
1:F:47:G:N3	1:F:47:G:H2'	2.33	0.43
2:A:130:ALA:HB2	2:B:96:ALA:HB3	2.00	0.43
2:A:132:LEU:HD23	2:A:136:VAL:CG1	2.47	0.43
1:F:38:A:H2'	1:F:39:U:C6	2.54	0.43
2:C:64:HIS:HE1	2:C:135:GLY:HA2	1.83	0.43
2:D:223:TRP:CZ2	2:D:227:LEU:HD11	2.54	0.43
2:A:165:ARG:HD2	2:A:200:VAL:CG1	2.49	0.43
2:A:41:LYS:O	2:A:45:GLN:HG3	2.19	0.43
2:C:85:LEU:HD11	2:D:126:ARG:CZ	2.48	0.43
2:B:230:ALA:HB1	2:B:235:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:116:ARG:HD2	2:C:116:ARG:N	2.33	0.43
2:C:186:HIS:O	2:C:189:TYR:N	2.44	0.43
2:A:172:ARG:CZ	2:A:172:ARG:HB2	2.49	0.43
2:A:173:THR:HG23	2:A:173:THR:O	2.18	0.43
2:A:46:VAL:HG12	2:A:78:ARG:HG3	2.01	0.42
2:B:116:ARG:HD2	2:B:116:ARG:N	2.34	0.42
2:B:261:PRO:HB2	2:B:262:PRO:HD2	1.99	0.42
2:A:165:ARG:HD2	2:A:200:VAL:CB	2.49	0.42
2:D:64:HIS:CE1	2:D:135:GLY:HA2	2.54	0.42
2:C:85:LEU:HD23	2:D:127:LEU:CD2	2.48	0.42
1:F:16:U:H2'	1:F:16:U:O2	2.20	0.42
2:B:158:GLU:HG2	2:B:177:ASN:CB	2.50	0.42
2:A:141:GLU:HA	2:A:142:PRO:HD3	1.80	0.42
2:B:46:VAL:HG12	2:B:78:ARG:HG3	2.00	0.42
2:D:78:ARG:HH11	2:D:78:ARG:HG2	1.85	0.42
2:C:167:VAL:C	2:C:169:CYS:N	2.72	0.42
2:B:132:LEU:HD23	2:B:136:VAL:CG1	2.48	0.42
2:C:63:VAL:CG2	2:C:245:LEU:HD23	2.50	0.42
1:F:58:A:C2	1:F:61:C:C6	3.08	0.42
2:D:42:ALA:HA	2:D:45:GLN:NE2	2.34	0.42
1:F:6:G:H2'	1:F:7:A:O4'	2.19	0.42
2:A:121:ILE:HD11	2:A:268:LEU:CD1	2.50	0.42
2:C:107:PHE:CE1	2:C:258:LEU:HD11	2.55	0.42
2:C:92:PRO:HB2	2:C:94:ASP:OD1	2.20	0.41
2:C:99:TRP:O	2:C:99:TRP:CE3	2.73	0.41
2:B:179:MET:N	2:B:195:LYS:O	2.51	0.41
2:D:116:ARG:N	2:D:116:ARG:HD2	2.35	0.41
1:F:60:U:C5'	1:F:61:C:OP2	2.64	0.41
2:A:99:TRP:CE2	2:A:259:PRO:HG2	2.55	0.41
2:A:100:VAL:HG22	2:A:101:LYS:N	2.35	0.41
2:B:63:VAL:CG2	2:B:245:LEU:HD23	2.50	0.41
2:D:46:VAL:HG12	2:D:78:ARG:HG3	2.02	0.41
2:A:119:ARG:HD2	2:A:248:VAL:HG11	2.01	0.41
1:F:15:A:H2	1:F:20(A):A:H1'	1.85	0.41
2:B:100:VAL:HG22	2:B:101:LYS:N	2.36	0.41
2:D:268:LEU:HD23	2:D:268:LEU:HA	1.94	0.41
2:D:149:HIS:CE1	2:D:153:GLN:NE2	2.88	0.41
2:B:141:GLU:HA	2:B:142:PRO:HD3	1.82	0.41
2:C:179:MET:N	2:C:195:LYS:O	2.49	0.41
2:A:255:ARG:HG3	2:A:256:TYR:N	2.36	0.41
2:B:255:ARG:HG3	2:B:256:TYR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:59:THR:HB	2:A:63:VAL:HB	2.02	0.41
2:C:56:ALA:HB2	2:C:252:TYR:OH	2.21	0.41
2:A:12:ILE:O	2:A:71:HIS:HA	2.20	0.41
2:D:165:ARG:CG	2:D:166:ALA:H	2.18	0.41
2:D:233:ARG:C	2:D:235:LEU:N	2.73	0.41
2:C:223:TRP:CZ2	2:C:227:LEU:HD11	2.55	0.41
2:A:170:GLN:HE21	2:A:170:GLN:HB3	1.72	0.41
2:A:79:LYS:O	2:A:80:ASP:C	2.58	0.41
1:F:24:A:C5	1:F:25:C:C5	3.09	0.41
2:B:233:ARG:C	2:B:235:LEU:N	2.74	0.41
1:F:18:G:C6	1:F:57:A:N6	2.89	0.41
2:D:123:TYR:CE2	2:D:129:PRO:HB3	2.56	0.41
2:B:268:LEU:HA	2:B:268:LEU:HD23	1.91	0.41
2:B:120:TYR:CD1	2:B:208:VAL:HG11	2.56	0.41
2:D:158:GLU:HG2	2:D:177:ASN:CB	2.51	0.41
2:A:26:TRP:O	2:A:34:SER:HB2	2.21	0.41
2:B:9:VAL:HG12	2:B:73:GLU:HB3	2.02	0.41
2:C:121:ILE:HD11	2:C:268:LEU:CD1	2.51	0.41
2:C:128:ARG:NH1	2:D:93:GLY:HA2	2.36	0.41
2:D:255:ARG:HG3	2:D:256:TYR:N	2.36	0.41
2:A:148:MET:HE3	2:A:211:LEU:O	2.20	0.41
2:B:123:TYR:CE2	2:B:129:PRO:HB3	2.56	0.40
2:A:268:LEU:HA	2:A:268:LEU:HD23	1.93	0.40
2:D:100:VAL:HG22	2:D:101:LYS:N	2.36	0.40
2:B:43:LEU:HD23	2:B:87:VAL:CG2	2.51	0.40
2:D:56:ALA:HB2	2:D:252:TYR:OH	2.22	0.40
2:D:266:LEU:HB3	2:D:267:PHE:H	1.66	0.40
1:F:12:G:H3'	1:F:13:G:H8	1.87	0.40
2:C:59:THR:HB	2:C:63:VAL:HB	2.03	0.40
2:A:47:ALA:HB2	2:A:83:TRP:HH2	1.86	0.40
2:D:99:TRP:CE3	2:D:99:TRP: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	
2	A	260/270 (96%)	230 (88%)	28 (11%)	2 (1%)	24	70
2	B	262/270 (97%)	228 (87%)	31 (12%)	3 (1%)	17	63
2	C	262/270 (97%)	229 (87%)	29 (11%)	4 (2%)	13	56
2	D	261/270 (97%)	226 (87%)	31 (12%)	4 (2%)	13	56
All	All	1045/1080 (97%)	913 (87%)	119 (11%)	13 (1%)	16	61

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	243	GLU
2	B	243	GLU
2	C	243	GLU
2	D	243	GLU
2	C	168	GLN
2	A	234	THR
2	B	234	THR
2	C	31	GLU
2	C	234	THR
2	D	234	THR
2	B	31	GLU
2	D	30	ASN
2	D	244	GLY

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	
2	A	214/223 (96%)	200 (94%)	14 (6%)	21	62
2	B	214/223 (96%)	198 (92%)	16 (8%)	17	55
2	C	207/223 (93%)	198 (96%)	9 (4%)	35	74
2	D	216/223 (97%)	198 (92%)	18 (8%)	14	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	851/892 (95%)	794 (93%)	57 (7%)	20 61

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	31	GLU
2	A	58	ARG
2	A	77	LEU
2	A	94	ASP
2	A	114	THR
2	A	156	LEU
2	A	163	SER
2	A	167	VAL
2	A	168	GLN
2	A	170	GLN
2	A	172	ARG
2	A	179	MET
2	A	233	ARG
2	A	251	ASP
2	B	30	ASN
2	B	33	ARG
2	B	41	LYS
2	B	58	ARG
2	B	77	LEU
2	B	79	LYS
2	B	114	THR
2	B	156	LEU
2	B	163	SER
2	B	165	ARG
2	B	168	GLN
2	B	172	ARG
2	B	173	THR
2	B	179	MET
2	B	233	ARG
2	B	251	ASP
2	C	58	ARG
2	C	77	LEU
2	C	114	THR
2	C	156	LEU
2	C	163	SER
2	C	165	ARG
2	C	179	MET

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Mol	Chain	Res	Type
2	C	233	ARG
2	C	251	ASP
2	D	27	GLN
2	D	29	GLN
2	D	31	GLU
2	D	41	LYS
2	D	58	ARG
2	D	77	LEU
2	D	79	LYS
2	D	94	ASP
2	D	114	THR
2	D	156	LEU
2	D	163	SER
2	D	168	GLN
2	D	170	GLN
2	D	171	SER
2	D	172	ARG
2	D	179	MET
2	D	233	ARG
2	D	251	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	29	GLN
2	A	30	ASN
2	A	45	GLN
2	A	64	HIS
2	A	124	ASN
2	A	125	HIS
2	A	153	GLN
2	A	168	GLN
2	A	170	GLN
2	A	182	ASN
2	A	218	ASN
2	B	30	ASN
2	B	36	GLN
2	B	45	GLN
2	B	124	ASN
2	B	125	HIS
2	B	153	GLN
2	B	159	ASN

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Mol	Chain	Res	Type
2	B	170	GLN
2	B	182	ASN
2	B	218	ASN
2	C	36	GLN
2	C	45	GLN
2	C	64	HIS
2	C	90	ASN
2	C	124	ASN
2	C	125	HIS
2	C	153	GLN
2	C	159	ASN
2	C	182	ASN
2	C	218	ASN
2	D	27	GLN
2	D	45	GLN
2	D	64	HIS
2	D	124	ASN
2	D	125	HIS
2	D	153	GLN
2	D	168	GLN
2	D	182	ASN
2	D	218	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	F	65/87 (74%)	14 (21%)	3 (4%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	F	7	A
1	F	9	G
1	F	10	G
1	F	14	A
1	F	17	C
1	F	18	G
1	F	19	G
1	F	20	U
1	F	20(A)	A
1	F	45(D)	G

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Mol	Chain	Res	Type
1	F	49	G
1	F	51	G
1	F	59	G
1	F	61	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	F	18	G
1	F	58	A
1	F	60	U

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	F	71/87 (81%)	0.66	6 (8%) 13 12	27, 80, 197, 241	5 (7%)
2	A	264/270 (97%)	-0.41	0 100 100	8, 18, 43, 60	0
2	B	264/270 (97%)	-0.41	0 100 100	8, 21, 42, 64	0
2	C	264/270 (97%)	-0.08	1 (0%) 93 90	8, 34, 67, 81	0
2	D	263/270 (97%)	-0.09	1 (0%) 93 90	10, 30, 53, 76	5 (1%)
All	All	1126/1167 (96%)	-0.19	8 (0%) 89 82	8, 27, 67, 241	10 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	70	G	7.2
1	F	3	C	2.8
1	F	67	C	2.7
2	D	8	PRO	2.7
1	F	45(D)	G	2.2
2	C	232	ASP	2.2
1	F	46(K)	C	2.1
1	F	66	U	2.0

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	K	F	79	1/1	0.94	0.21	-	74,74,74,74	0
3	K	F	78	1/1	0.96	0.15	-	28,28,28,28	0
3	K	F	81	1/1	0.62	0.33	-	67,67,67,67	0
3	K	C	271	1/1	0.89	0.14	-	26,26,26,26	0
3	K	F	80	1/1	0.88	0.11	-	72,72,72,72	0
3	K	F	77	1/1	0.61	0.77	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.