Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:16 am BST

PDB ID	:	5LM7
Title	:	Crystal structure of the lambda N-Nus factor complex
Authors	:	Said, N.; Santos, K.; Weber, G.; Wahl, M.C.
Deposited on	:	2016-07-29
Resolution	:	3.35 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 following versions of software and data (see references ①) were used in the production of this report:

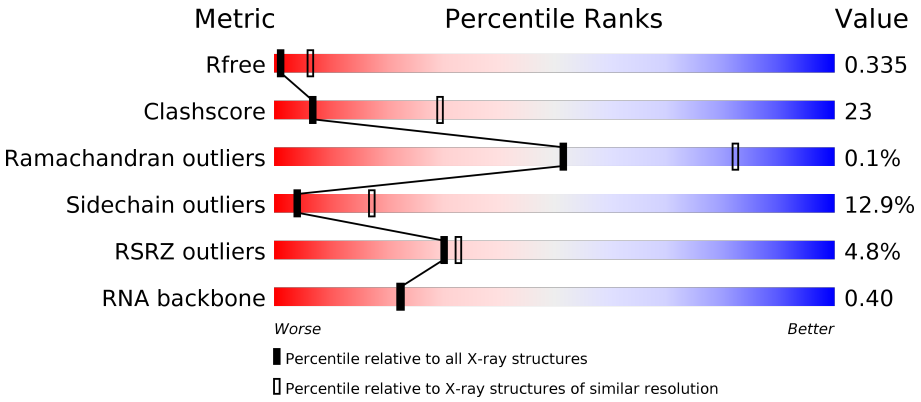
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	3% 50% 42% 7%
1	C	428	4% 56% 37% 6%
2	B	141	6% 33% 51% 11% 5%
2	D	141	6% 50% 39% 6%

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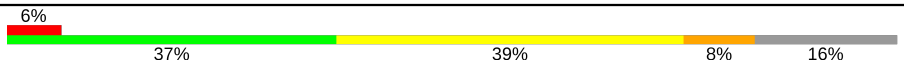
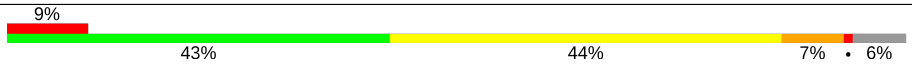
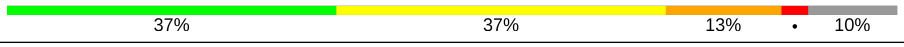
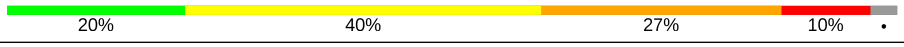
Mol	Chain	Length	Quality of chain
3	E	108	
3	J	108	
4	F	89	
4	N	89	
5	G	30	
5	R	30	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3345	2082	585	668	10			
1	C	423	Total	C	N	O	S	0	0	0
			3308	2061	580	657	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P0AFF8
A	0	ALA	-	expression tag	UNP P0AFF8
C	-1	GLY	-	expression tag	UNP P0AFF8
C	0	ALA	-	expression tag	UNP P0AFF8

- Molecule 2 is a protein called N utilization substance protein B homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1063	677	183	201	2			
2	D	132	Total	C	N	O	S	0	0	0
			1050	670	180	198	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP B7MD74
B	0	ALA	-	expression tag	UNP B7MD74
D	-1	GLY	-	expression tag	UNP B7MD74
D	0	ALA	-	expression tag	UNP B7MD74

- Molecule 3 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	96	Total	C	N	O	S	0	0	0
			771	482	147	141	1			
3	E	91	Total	C	N	O	S	0	0	0
			733	459	139	134	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	GLY	-	expression tag	UNP B7MCT6
J	-3	PRO	-	expression tag	UNP B7MCT6
J	-2	LEU	-	expression tag	UNP B7MCT6
J	-1	GLY	-	expression tag	UNP B7MCT6
J	0	SER	-	expression tag	UNP B7MCT6
E	-4	GLY	-	expression tag	UNP B7MCT6
E	-3	PRO	-	expression tag	UNP B7MCT6
E	-2	LEU	-	expression tag	UNP B7MCT6
E	-1	GLY	-	expression tag	UNP B7MCT6
E	0	SER	-	expression tag	UNP B7MCT6

- Molecule 4 is a protein called Antitermination protein N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	85	Total	C	N	O	S	0	0	0
			693	428	141	123	1			
4	F	84	Total	C	N	O	S	0	0	0
			679	417	139	122	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-4	GLY	-	expression tag	UNP P03045
N	-3	PRO	-	expression tag	UNP P03045
N	-2	LEU	-	expression tag	UNP P03045
N	-1	GLY	-	expression tag	UNP P03045
N	0	SER	-	expression tag	UNP P03045
F	-4	GLY	-	expression tag	UNP P03045
F	-3	PRO	-	expression tag	UNP P03045
F	-2	LEU	-	expression tag	UNP P03045
F	-1	GLY	-	expression tag	UNP P03045
F	0	SER	-	expression tag	UNP P03045

- Molecule 5 is a RNA chain called RNA (29-MER).

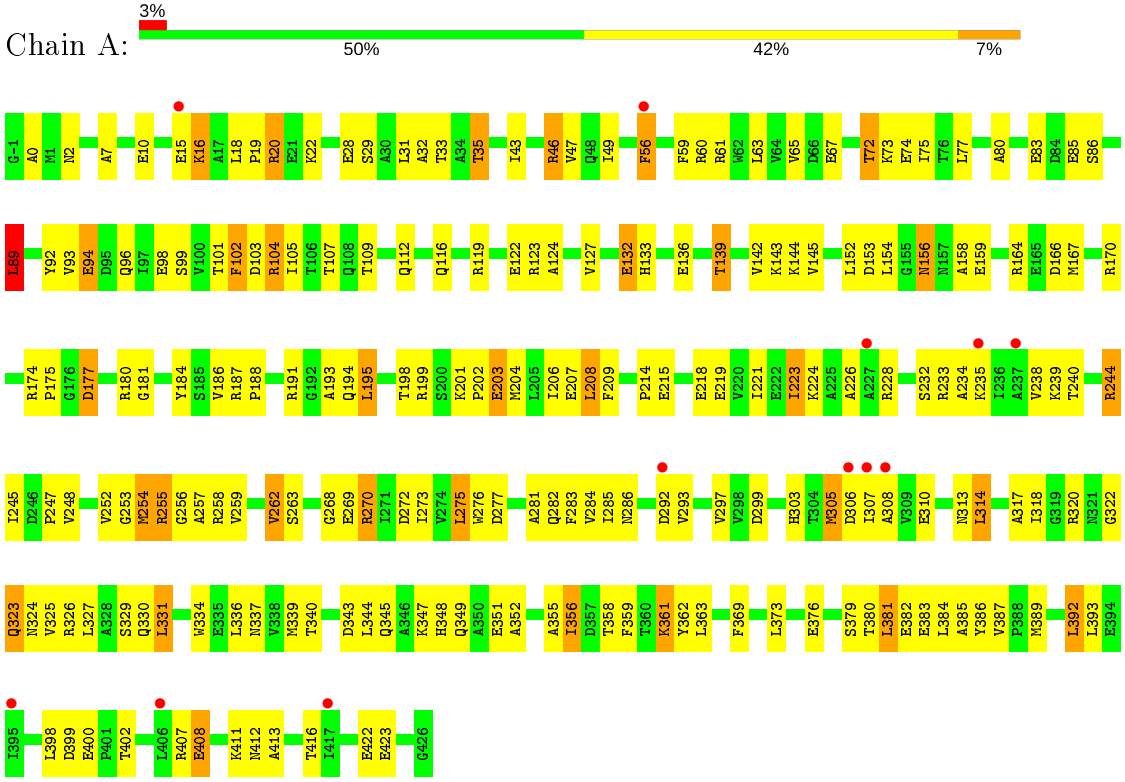
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	29	Total	C	N	O	P	0	0	0
			616	276	110	201	29			
5	G	27	Total	C	N	O	P	0	0	0
			576	258	105	186	27			

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

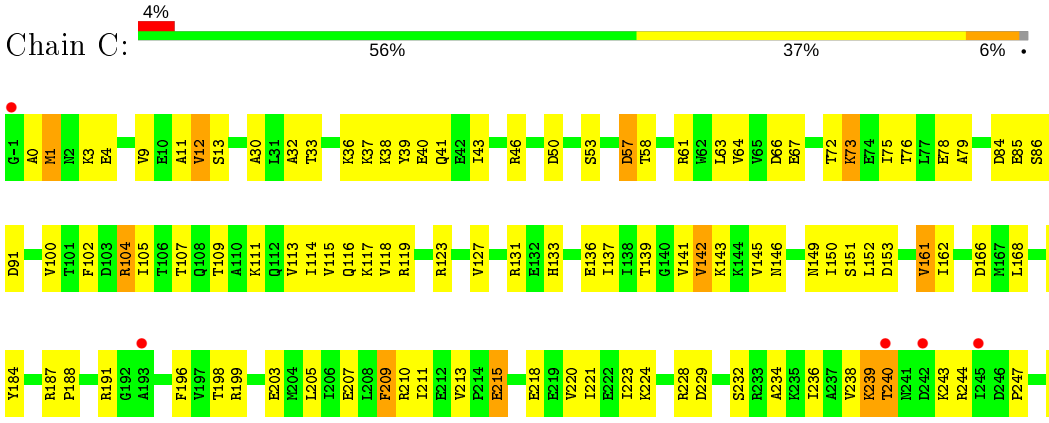
- Molecule 1: Transcription termination/antitermination protein NusA

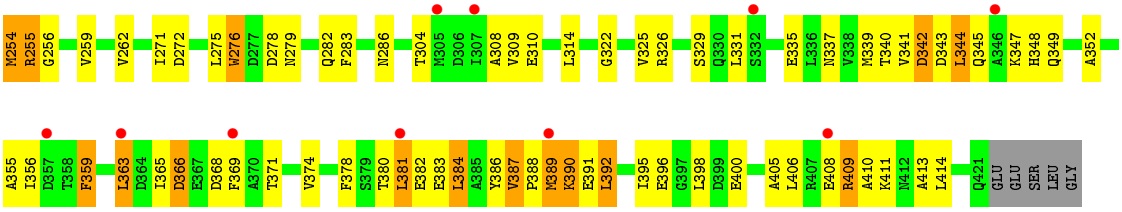
Chain A:



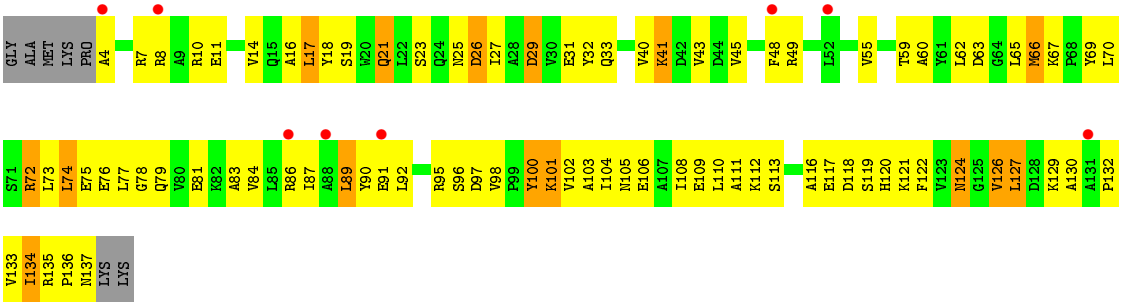
- Molecule 1: Transcription termination/antitermination protein NusA

Chain C:

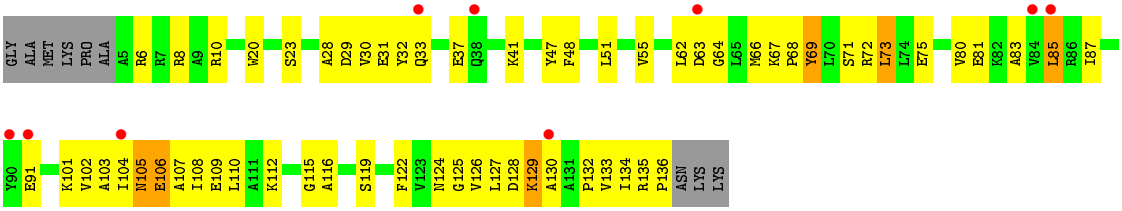




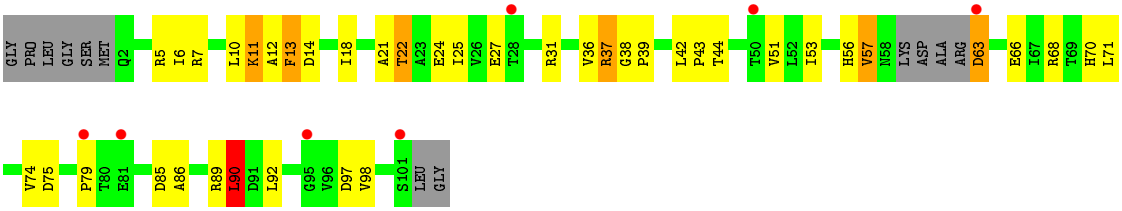
• Molecule 2: N utilization substance protein B homolog



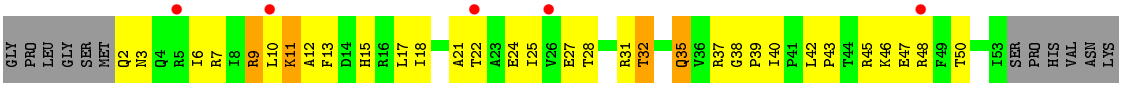
• Molecule 2: N utilization substance protein B homolog

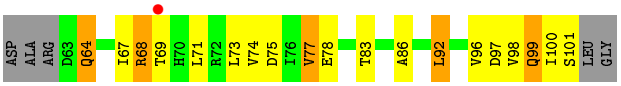


• Molecule 3: 30S ribosomal protein S10



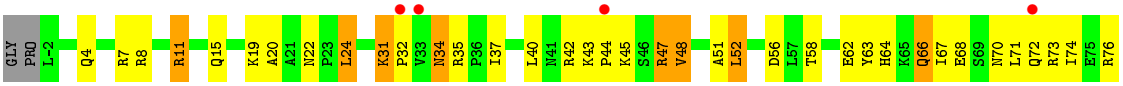
• Molecule 3: 30S ribosomal protein S10

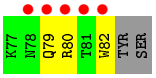




- Molecule 4: Antitermination protein N

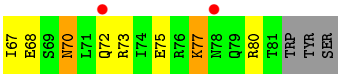
Chain N:





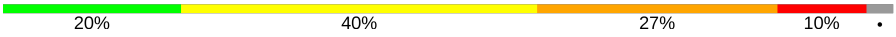
- Molecule 4: Antitermination protein N

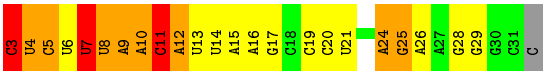
Chain F:



- Molecule 5: RNA (29-MER)

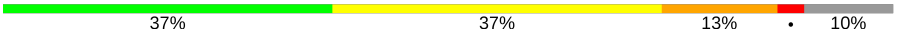
Chain R:





- Molecule 5: RNA (29-MER)

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.78Å 101.80Å 279.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.52 – 3.35 48.33 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.52-3.35) 99.4 (48.33-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.297 , 0.335 0.298 , 0.335	Depositor DCC
R_{free} test set	2004 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	117.5	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 110.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12834	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/3385	0.51	2/4578 (0.0%)
1	C	0.28	0/3348	0.49	1/4530 (0.0%)
2	B	0.34	0/1080	0.56	0/1462
2	D	0.27	0/1067	0.46	0/1444
3	E	0.28	0/740	0.49	0/999
3	J	0.26	0/780	0.56	1/1055 (0.1%)
4	F	0.26	0/687	0.56	1/923 (0.1%)
4	N	0.28	0/703	0.52	0/946
5	G	0.31	0/644	1.06	2/1001 (0.2%)
5	R	0.46	0/688	1.24	6/1069 (0.6%)
All	All	0.29	0/13122	0.62	13/18007 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	3	C	N1-C2-O2	9.01	124.30	118.90
5	R	7	U	N1-C2-O2	7.61	128.13	122.80
5	R	7	U	N3-C2-O2	-7.04	117.28	122.20
3	J	90	LEU	CA-CB-CG	6.85	131.04	115.30
5	G	7	U	C2-N1-C1'	6.80	125.86	117.70
5	R	7	U	C2-N1-C1'	6.62	125.64	117.70
5	R	3	C	N3-C2-O2	-5.80	117.84	121.90
1	A	89	LEU	CA-CB-CG	5.66	128.32	115.30
5	G	7	U	C6-N1-C1'	-5.54	113.45	121.20
4	F	24	LEU	CA-CB-CG	5.52	128.00	115.30
5	R	11	C	P-O3'-C3'	5.43	126.22	119.70
1	A	314	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	344	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3345	0	3346	180	0
1	C	3308	0	3315	148	0
2	B	1063	0	1071	87	0
2	D	1050	0	1060	45	0
3	E	733	0	769	42	0
3	J	771	0	803	33	0
4	F	679	0	719	45	0
4	N	693	0	729	44	0
5	G	576	0	292	19	0
5	R	616	0	313	38	0
All	All	12834	0	12417	581	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 23.

All (581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:85:ASP:O	3:J:89:ARG:HB2	1.54	1.07
2:B:62:LEU:HD13	2:B:89:LEU:HB3	1.41	1.01
1:A:244:ARG:HG3	1:A:245:ILE:HG13	1.50	0.91
2:B:92:LEU:HD21	2:B:133:VAL:HG11	1.49	0.91
4:N:24:LEU:HD22	4:N:24:LEU:H	1.36	0.90
2:B:109:GLU:HA	2:B:112:LYS:HG3	1.55	0.88
1:A:61:ARG:HA	1:A:94:GLU:HG2	1.59	0.85
1:C:363:LEU:HD21	1:C:365:ILE:HG12	1.57	0.84
4:F:18:TRP:O	4:F:22:ASN:ND2	2.10	0.84
4:F:24:LEU:HD11	4:F:26:VAL:HG13	1.60	0.83
2:B:108:ILE:HD11	2:B:127:LEU:HD11	1.58	0.83
2:B:62:LEU:HB2	2:B:89:LEU:HD22	1.61	0.82
3:J:12:ALA:HB1	3:J:18:ILE:HG13	1.60	0.82
1:C:259:VAL:HG21	5:G:12:A:H8	1.44	0.81
1:A:320:ARG:NH1	5:R:16:A:OP2	2.15	0.79
2:B:133:VAL:HG13	2:B:134:ILE:HG12	1.66	0.78
2:D:72:ARG:NH1	5:G:8:U:OP2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:LEU:HA	1:C:384:LEU:HD21	1.66	0.78
2:B:124:ASN:ND2	2:B:124:ASN:O	2.17	0.77
1:C:142:VAL:HA	1:C:152:LEU:HA	1.65	0.77
2:D:122:PHE:HA	5:G:7:U:H1'	1.67	0.76
1:A:330:GLN:O	4:N:35:ARG:NH1	2.18	0.76
1:A:422:GLU:HG3	1:A:423:GLU:HG2	1.69	0.75
2:D:37:GLU:OE1	3:E:7:ARG:NH1	2.20	0.75
1:A:188:PRO:HA	1:A:193:ALA:HB2	1.67	0.75
1:A:299:ASP:O	1:A:303:HIS:N	2.16	0.74
1:A:282:GLN:O	1:A:286:ASN:ND2	2.21	0.74
1:C:220:VAL:HG13	1:C:243:LYS:HD2	1.69	0.74
2:B:73:LEU:HB2	2:B:76:GLU:HB2	1.69	0.73
1:C:380:THR:OG1	1:C:382:GLU:OE2	2.07	0.72
1:A:221:ILE:HG22	1:A:240:THR:HB	1.71	0.72
2:D:104:ILE:HG21	2:D:127:LEU:HD13	1.72	0.72
1:A:204:MET:O	1:A:208:LEU:HB2	1.90	0.72
1:A:352:ALA:HB1	1:A:373:LEU:HD21	1.72	0.72
1:C:239:LYS:HG2	1:C:276:TRP:CE3	2.25	0.71
1:C:50:ASP:HB3	1:C:53:SER:HB3	1.71	0.71
1:C:180:ARG:O	1:C:199:ARG:NH1	2.24	0.71
1:C:398:LEU:HD11	1:C:400:GLU:HG3	1.71	0.71
1:A:259:VAL:HG11	5:R:12:A:H8	1.57	0.70
1:A:85:GLU:O	1:C:187:ARG:NH1	2.25	0.70
2:B:69:TYR:H	2:B:129:LYS:HZ1	1.39	0.70
2:B:110:LEU:O	2:B:113:SER:OG	2.09	0.69
1:C:366:ASP:N	1:C:366:ASP:OD1	2.25	0.69
2:B:130:ALA:O	2:B:133:VAL:HG12	1.92	0.68
2:B:7:ARG:HB3	2:B:10:ARG:HH21	1.58	0.68
4:F:24:LEU:HD22	4:F:25:LEU:N	2.07	0.68
1:A:292:ASP:O	1:A:313:ASN:ND2	2.26	0.68
1:A:320:ARG:HH22	5:R:16:A:H3'	1.58	0.68
2:B:59:THR:HA	2:B:62:LEU:HG	1.76	0.67
1:A:387:VAL:O	1:A:407:ARG:NH2	2.25	0.67
1:A:208:LEU:HD12	1:A:262:VAL:HB	1.76	0.66
4:N:7:ARG:NH1	5:R:21:U:OP2	2.28	0.66
1:C:141:VAL:O	1:C:153:ASP:N	2.28	0.66
1:A:156:ASN:ND2	4:N:56:ASP:OD1	2.28	0.66
1:A:408:GLU:HA	1:A:411:LYS:HE2	1.78	0.66
1:C:32:ALA:O	1:C:36:LYS:HB2	1.96	0.66
1:A:275:LEU:HD12	1:A:275:LEU:H	1.61	0.65
3:E:3:ASN:ND2	3:E:78:GLU:OE1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:LEU:HA	3:E:11:LYS:HE2	1.79	0.65
2:B:111:ALA:HB3	2:B:120:HIS:HB3	1.78	0.65
3:J:11:LYS:HG2	3:J:97:ASP:HB2	1.77	0.64
1:A:2:ASN:ND2	1:A:107:THR:OG1	2.31	0.64
1:C:259:VAL:HG21	5:G:12:A:C8	2.30	0.64
3:E:9:ARG:HG3	3:E:73:LEU:HD13	1.79	0.64
2:B:117:GLU:HG2	5:R:9:A:O4'	1.97	0.64
2:B:26:ASP:OD1	2:B:26:ASP:N	2.31	0.63
2:D:23:SER:OG	3:E:38:GLY:O	2.16	0.63
3:J:18:ILE:O	3:J:22:THR:OG1	2.16	0.63
4:N:63:TYR:CZ	4:N:67:ILE:HD11	2.33	0.63
1:A:49:ILE:HG13	1:A:56:PHE:HB3	1.80	0.63
3:E:12:ALA:HB2	3:E:96:VAL:HG13	1.80	0.62
1:C:282:GLN:O	1:C:286:ASN:ND2	2.32	0.62
2:B:40:VAL:HB	2:B:43:VAL:HG22	1.81	0.62
1:A:199:ARG:O	1:A:228:ARG:NH2	2.32	0.62
1:A:89:LEU:HD12	1:C:188:PRO:HB3	1.82	0.62
1:C:203:GLU:N	1:C:203:GLU:OE1	2.33	0.62
2:B:102:VAL:HA	5:R:3:C:O2'	2.00	0.62
3:J:63:ASP:N	3:J:63:ASP:OD1	2.32	0.62
1:A:166:ASP:HB3	1:A:198:THR:HA	1.82	0.61
1:C:66:ASP:OD1	1:C:67:GLU:N	2.31	0.61
1:A:320:ARG:HH12	5:R:16:A:H5"	1.65	0.61
2:B:84:VAL:HA	2:B:87:ILE:HD12	1.81	0.61
2:B:120:HIS:CE1	2:B:121:LYS:HG3	2.35	0.61
5:R:20:C:H42	5:R:28:G:H1	1.49	0.61
1:C:387:VAL:HG22	1:C:388:PRO:HD2	1.82	0.61
2:B:120:HIS:CD2	2:B:120:HIS:H	2.17	0.61
4:F:75:GLU:OE1	4:F:80:ARG:NH2	2.28	0.61
1:A:63:LEU:HA	1:A:92:TYR:HB2	1.83	0.61
1:C:344:LEU:O	1:C:348:HIS:ND1	2.32	0.61
1:C:232:SER:OG	5:G:16:A:N6	2.34	0.60
4:F:8:ARG:NH2	4:F:15:GLN:OE1	2.34	0.60
2:D:112:LYS:O	3:E:68:ARG:NH1	2.35	0.60
1:C:347:LYS:NZ	4:F:22:ASN:O	2.27	0.60
4:N:66:GLN:O	4:N:70:ASN:ND2	2.27	0.60
1:C:396:GLU:N	1:C:396:GLU:OE1	2.34	0.60
1:C:87:LEU:HD12	1:C:91:ASP:HB3	1.84	0.60
1:A:223:ILE:H	1:A:223:ILE:HD13	1.67	0.60
5:G:7:U:O2'	5:G:8:U:H5'	2.01	0.60
2:B:31:GLU:OE1	2:B:49:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ASP:N	1:C:368:ASP:OD1	2.34	0.60
1:C:344:LEU:HD12	1:C:345:GLN:N	2.17	0.59
1:C:139:THR:HG22	1:C:180:ARG:HG2	1.84	0.59
1:A:139:THR:HG23	1:A:180:ARG:HG3	1.85	0.59
2:B:74:LEU:HD13	2:B:74:LEU:H	1.68	0.59
2:B:132:PRO:HA	2:B:135:ARG:HH11	1.67	0.59
1:A:254:MET:HG3	1:A:257:ALA:HB3	1.84	0.58
2:B:109:GLU:OE1	5:R:5:C:N4	2.36	0.58
1:C:133:HIS:HE1	4:F:53:ASN:HB3	1.68	0.58
1:C:1:MET:N	1:C:1:MET:SD	2.77	0.58
4:N:62:GLU:O	4:N:66:GLN:NE2	2.36	0.58
2:B:17:LEU:O	2:B:21:GLN:N	2.29	0.58
4:F:7:ARG:HG2	4:F:10:ARG:HH21	1.68	0.58
2:B:14:VAL:HG22	2:B:87:ILE:HD13	1.84	0.58
2:B:72:ARG:HE	2:B:72:ARG:HA	1.69	0.58
4:F:63:TYR:CZ	4:F:67:ILE:HD11	2.39	0.58
4:N:4:GLN:NE2	5:R:25:G:OP1	2.32	0.58
1:A:253:GLY:HA3	1:A:258:ARG:HB2	1.85	0.57
4:N:34:ASN:O	4:N:34:ASN:ND2	2.37	0.57
1:A:240:THR:HG22	1:A:247:PRO:HD3	1.85	0.57
1:A:103:ASP:OD1	1:A:104:ARG:N	2.32	0.57
1:A:277:ASP:HB3	1:A:283:PHE:HB2	1.85	0.57
2:B:69:TYR:H	2:B:129:LYS:NZ	2.01	0.57
1:C:12:VAL:HG21	1:C:118:VAL:HG21	1.85	0.57
3:E:7:ARG:HA	3:E:75:ASP:HA	1.85	0.57
1:A:318:ILE:HG21	5:R:25:G:N3	2.19	0.57
1:A:180:ARG:O	1:A:199:ARG:NH2	2.38	0.57
3:E:28:THR:O	3:E:32:THR:OG1	2.22	0.57
2:D:127:LEU:HA	2:D:130:ALA:HB3	1.85	0.57
1:C:253:GLY:O	5:G:10:A:O2'	2.22	0.57
1:C:255:ARG:NH2	5:G:12:A:OP1	2.37	0.57
2:D:67:LYS:N	2:D:68:PRO:HD2	2.19	0.57
1:A:181:GLY:HA2	1:A:204:MET:HE1	1.84	0.57
1:A:340:THR:OG1	1:A:343:ASP:OD1	2.23	0.57
1:C:0:ALA:HA	1:C:3:LYS:HE3	1.87	0.57
1:C:386:TYR:OH	1:C:409:ARG:NH1	2.37	0.57
4:F:20:ALA:O	4:F:22:ASN:ND2	2.38	0.57
3:E:28:THR:HG22	4:F:48:VAL:HG13	1.86	0.57
4:F:49:GLU:O	4:F:53:ASN:N	2.38	0.57
1:C:57:ASP:OD1	1:C:57:ASP:N	2.38	0.57
2:B:116:ALA:HA	3:J:68:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ARG:HB3	1:C:123:ARG:NH1	2.20	0.57
3:J:7:ARG:NH2	3:J:75:ASP:OD1	2.38	0.57
3:J:10:LEU:HD23	3:J:98:VAL:HG12	1.86	0.56
1:A:20:ARG:H	1:A:20:ARG:NE	2.03	0.56
1:A:224:LYS:HG3	1:A:276:TRP:CG	2.40	0.56
1:C:405:ALA:O	1:C:408:GLU:HB3	2.05	0.56
2:D:107:ALA:HA	2:D:110:LEU:HD23	1.86	0.56
1:A:297:VAL:O	1:A:305:MET:HB2	2.05	0.56
1:C:276:TRP:HB2	1:C:283:PHE:CD1	2.41	0.56
1:C:363:LEU:HG	1:C:365:ILE:HG23	1.86	0.56
3:J:14:ASP:O	3:J:18:ILE:HG12	2.04	0.56
2:B:118:ASP:HB3	2:B:121:LYS:HD2	1.86	0.56
1:C:348:HIS:O	1:C:352:ALA:HB2	2.05	0.56
5:R:7:U:O2	5:R:7:U:H2'	2.04	0.56
2:B:45:VAL:HA	2:B:48:PHE:HB3	1.86	0.56
1:C:205:LEU:HG	1:C:236:ILE:HD11	1.87	0.56
1:C:30:ALA:O	1:C:33:THR:OG1	2.15	0.56
2:D:29:ASP:O	2:D:33:GLN:HG2	2.05	0.56
1:A:320:ARG:NH2	5:R:16:A:N3	2.54	0.56
1:C:133:HIS:CE1	4:F:53:ASN:HB3	2.41	0.56
2:D:68:PRO:HB2	2:D:129:LYS:HE2	1.88	0.56
1:A:323:GLN:HA	1:A:326:ARG:HB3	1.88	0.56
1:A:330:GLN:OE1	4:N:35:ARG:NH1	2.38	0.56
1:C:223:ILE:HG22	1:C:238:VAL:HB	1.88	0.56
1:C:224:LYS:HB2	1:C:276:TRP:CZ3	2.41	0.56
2:B:104:ILE:HG13	2:B:127:LEU:HD22	1.87	0.55
3:E:47:GLU:HG2	3:E:69:THR:HG21	1.87	0.55
1:A:206:ILE:HD11	1:A:226:ALA:HB2	1.87	0.55
1:C:207:GLU:OE2	1:C:210:ARG:NH1	2.40	0.55
1:C:339:MET:HB3	1:C:343:ASP:HB2	1.87	0.55
2:D:102:VAL:O	2:D:106:GLU:HB3	2.06	0.55
1:A:195:LEU:H	1:A:195:LEU:HD22	1.71	0.55
1:A:259:VAL:HG11	5:R:12:A:C8	2.40	0.55
2:B:29:ASP:N	2:B:29:ASP:OD1	2.38	0.55
3:J:36:VAL:HG22	3:J:37:ARG:H	1.72	0.55
1:A:363:LEU:HB3	1:A:369:PHE:CZ	2.42	0.55
2:B:67:LYS:HE3	2:B:74:LEU:HD12	1.89	0.55
1:A:0:ALA:HB2	1:A:102:PHE:CZ	2.42	0.55
3:J:56:HIS:CE1	3:J:57:VAL:HG13	2.40	0.55
1:A:156:ASN:HB2	4:N:56:ASP:HA	1.88	0.55
1:C:58:THR:HG22	1:C:100:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:11:C:O2'	5:R:12:A:OP2	2.20	0.54
1:A:98:GLU:OE1	1:A:99:SER:N	2.37	0.54
3:E:92:LEU:HD13	3:E:98:VAL:HG21	1.89	0.54
1:A:226:ALA:O	4:N:35:ARG:NH2	2.40	0.54
1:A:392:LEU:HD13	1:A:392:LEU:H	1.73	0.54
3:E:42:LEU:HG	3:E:43:PRO:HD2	1.90	0.54
1:A:297:VAL:HG21	1:A:348:HIS:NE2	2.23	0.54
1:C:127:VAL:O	1:C:131:ARG:HG2	2.08	0.54
1:C:308:ALA:HB2	1:C:344:LEU:HD23	1.90	0.54
2:D:125:GLY:HA3	5:G:7:U:C6	2.42	0.54
1:A:345:GLN:O	1:A:349:GLN:HG2	2.07	0.54
1:C:221:ILE:HG22	1:C:240:THR:HA	1.88	0.54
1:A:318:ILE:HG23	1:A:322:GLY:HA2	1.89	0.53
1:C:166:ASP:HB3	1:C:198:THR:HA	1.90	0.53
2:B:122:PHE:HB3	5:R:7:U:H4'	1.90	0.53
4:F:7:ARG:O	4:F:11:ARG:HG2	2.08	0.53
1:A:413:ALA:O	1:A:416:THR:OG1	2.17	0.53
2:D:105:ASN:ND2	5:G:5:C:OP1	2.40	0.53
1:C:215:GLU:HB2	1:C:221:ILE:HG12	1.91	0.53
2:B:98:VAL:HB	2:B:103:ALA:HB2	1.90	0.53
2:B:41:LYS:HD2	2:B:41:LYS:H	1.74	0.53
2:D:48:PHE:HA	2:D:51:LEU:HB3	1.90	0.53
1:C:50:ASP:OD1	1:C:53:SER:N	2.42	0.53
1:C:209:PHE:HE2	1:C:236:ILE:HD12	1.73	0.53
1:A:187:ARG:NH2	1:C:87:LEU:O	2.41	0.53
2:D:85:LEU:HD11	2:D:126:VAL:HG21	1.89	0.53
3:E:42:LEU:HD13	3:E:71:LEU:HD22	1.90	0.53
1:A:143:LYS:O	1:A:144:LYS:NZ	2.36	0.53
1:A:303:HIS:HB3	1:A:334:TRP:CE3	2.43	0.53
1:A:385:ALA:O	1:A:407:ARG:NH1	2.41	0.53
2:D:132:PRO:HA	2:D:135:ARG:NH1	2.24	0.53
2:B:105:ASN:OD1	5:R:5:C:N4	2.41	0.52
1:A:329:SER:HB2	1:A:336:LEU:HD23	1.89	0.52
1:A:239:LYS:HB2	1:A:276:TRP:HB3	1.90	0.52
1:A:320:ARG:O	1:A:323:GLN:NE2	2.37	0.52
1:A:393:LEU:HD22	1:A:399:ASP:HB2	1.91	0.52
2:D:51:LEU:HD21	2:D:87:ILE:HD13	1.90	0.52
2:D:109:GLU:HG2	5:G:5:C:H41	1.75	0.52
4:N:31:LYS:O	4:N:35:ARG:N	2.41	0.52
2:D:69:TYR:HB2	2:D:129:LYS:HD2	1.92	0.52
1:C:143:LYS:HB3	1:C:151:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ALA:HB1	3:E:15:HIS:CD2	2.45	0.52
3:E:50:THR:HA	3:E:64:GLN:HA	1.92	0.52
2:D:47:TYR:OH	2:D:91:GLU:OE1	2.28	0.52
3:E:32:THR:HB	3:E:83:THR:HG22	1.92	0.52
1:C:150:ILE:HD11	1:C:162:ILE:HD12	1.92	0.52
1:C:366:ASP:HB2	1:C:369:PHE:HD1	1.74	0.52
2:B:18:TYR:CE2	3:J:39:PRO:HG2	2.45	0.52
1:A:339:MET:SD	1:A:344:LEU:HD23	2.50	0.52
1:A:83:GLU:O	1:A:83:GLU:HG3	2.09	0.52
1:C:390:LYS:H	1:C:390:LYS:HD3	1.74	0.52
1:A:28:GLU:HB2	1:A:47:VAL:HG13	1.91	0.52
1:A:356:ILE:HG13	1:A:373:LEU:HD22	1.91	0.52
1:A:381:LEU:H	1:A:381:LEU:HD23	1.75	0.52
1:A:382:GLU:OE2	1:A:382:GLU:N	2.35	0.51
2:B:91:GLU:O	2:B:96:SER:N	2.38	0.51
1:C:104:ARG:HA	1:C:107:THR:HG22	1.91	0.51
1:C:392:LEU:HA	1:C:395:ILE:HG12	1.92	0.51
4:F:42:ARG:NH1	4:F:44:PRO:HB3	2.24	0.51
1:C:348:HIS:O	1:C:352:ALA:CB	2.58	0.51
1:C:411:LYS:O	1:C:414:LEU:HG	2.10	0.51
1:A:323:GLN:HB3	1:A:326:ARG:HH21	1.74	0.51
1:A:32:ALA:HB2	1:A:47:VAL:HG12	1.92	0.51
1:C:356:ILE:HD11	1:C:374:VAL:HG21	1.93	0.51
1:C:63:LEU:N	1:C:73:LYS:O	2.36	0.51
1:A:83:GLU:HG3	1:A:86:SER:HB2	1.91	0.51
2:B:100:TYR:O	2:B:104:ILE:HB	2.10	0.51
2:D:103:ALA:O	2:D:107:ALA:HB2	2.11	0.51
2:B:33:GLN:HG2	3:J:37:ARG:HD2	1.92	0.51
2:D:104:ILE:O	2:D:108:ILE:HG13	2.10	0.51
2:D:33:GLN:HB3	3:E:37:ARG:HD2	1.91	0.51
3:J:24:GLU:OE2	4:N:47:ARG:NH2	2.40	0.51
3:J:51:VAL:HG21	3:J:63:ASP:HA	1.93	0.51
2:B:16:ALA:O	2:B:19:SER:HB3	2.11	0.51
1:A:177:ASP:OD1	1:A:177:ASP:N	2.44	0.51
2:B:89:LEU:HA	2:B:92:LEU:HB3	1.93	0.51
1:A:187:ARG:NH2	1:C:85:GLU:O	2.43	0.50
1:A:63:LEU:HA	1:A:92:TYR:CB	2.41	0.50
5:R:10:A:H4'	5:R:11:C:OP2	2.11	0.50
3:E:46:LYS:HD2	3:E:48:ARG:HE	1.76	0.50
3:J:31:ARG:HG2	4:N:52:LEU:HD23	1.93	0.50
1:C:76:THR:OG1	1:C:78:GLU:OE1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ASP:O	2:D:67:LYS:N	2.44	0.50
3:J:42:LEU:HG	3:J:43:PRO:HD2	1.94	0.50
1:A:361:LYS:HA	1:A:361:LYS:HE3	1.94	0.50
1:A:77:LEU:HD12	1:A:80:ALA:HB3	1.94	0.50
3:E:46:LYS:HG3	3:E:67:ILE:O	2.12	0.50
1:A:282:GLN:HA	1:A:285:ILE:HD12	1.94	0.49
4:N:68:GLU:O	4:N:72:GLN:HG2	2.11	0.49
2:B:78:GLY:N	5:R:8:U:O4	2.43	0.49
1:A:94:GLU:CD	1:A:96:GLN:H	2.16	0.49
1:C:344:LEU:HD13	1:C:348:HIS:CE1	2.47	0.49
1:A:198:THR:OG1	1:A:201:LYS:HG2	2.13	0.49
1:A:276:TRP:HA	1:A:283:PHE:HE1	1.77	0.49
2:B:31:GLU:CD	2:B:49:ARG:HH22	2.14	0.49
2:B:4:ALA:O	2:B:8:ARG:N	2.38	0.49
1:C:105:ILE:O	1:C:109:THR:OG1	2.19	0.49
1:C:41:GLN:O	1:C:43:ILE:HG12	2.12	0.49
1:A:143:LYS:HD3	1:A:153:ASP:HB2	1.94	0.49
1:C:308:ALA:CB	1:C:344:LEU:HD23	2.43	0.49
3:E:9:ARG:HA	3:E:73:LEU:HA	1.95	0.49
1:A:214:PRO:O	1:A:218:GLU:N	2.33	0.49
1:A:235:LYS:NZ	1:A:272:ASP:OD2	2.46	0.49
1:A:282:GLN:HG3	1:A:286:ASN:HD21	1.78	0.49
4:N:43:LYS:N	4:N:44:PRO:HD2	2.27	0.49
1:C:304:THR:HG22	1:C:335:GLU:HB3	1.94	0.48
1:A:383:GLU:HA	1:A:386:TYR:HB2	1.94	0.48
2:B:60:ALA:HA	2:B:63:ASP:OD1	2.13	0.48
2:D:126:VAL:O	2:D:130:ALA:N	2.44	0.48
1:C:11:ALA:O	4:F:70:ASN:ND2	2.46	0.48
3:J:38:GLY:HA3	3:J:74:VAL:HG22	1.96	0.48
2:B:105:ASN:ND2	5:R:4:U:O5'	2.46	0.48
1:A:305:MET:HE2	1:A:305:MET:HB3	1.37	0.48
2:B:124:ASN:OD1	5:R:5:C:H6	1.96	0.48
1:C:388:PRO:HB2	1:C:391:GLU:OE1	2.13	0.48
4:F:68:GLU:O	4:F:72:GLN:HG2	2.14	0.48
1:A:244:ARG:NH2	2:B:73:LEU:HD23	2.29	0.48
3:J:44:THR:HG21	3:J:68:ARG:NE	2.29	0.48
4:N:76:ARG:HA	4:N:79:GLN:HB3	1.96	0.48
1:C:1:MET:HA	1:C:4:GLU:HB3	1.96	0.48
1:A:15:GLU:HB2	1:A:18:LEU:HD13	1.96	0.48
1:A:164:ARG:HA	1:A:167:MET:SD	2.54	0.47
1:A:174:ARG:HG2	1:A:175:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:LYS:HA	2:B:104:ILE:HG22	1.95	0.47
1:C:209:PHE:CE2	1:C:236:ILE:HD12	2.49	0.47
1:C:32:ALA:O	1:C:36:LYS:CB	2.62	0.47
1:A:0:ALA:HB2	1:A:102:PHE:CE2	2.49	0.47
1:A:142:VAL:HG22	1:A:152:LEU:HD22	1.95	0.47
1:A:293:VAL:HG21	1:A:307:ILE:HG23	1.96	0.47
3:E:21:ALA:O	3:E:25:ILE:HG12	2.13	0.47
4:N:8:ARG:NH2	5:R:25:G:O4'	2.46	0.47
1:A:244:ARG:HB2	1:A:244:ARG:HH11	1.80	0.47
1:A:29:SER:O	1:A:33:THR:OG1	2.28	0.47
2:D:115:GLY:HA3	2:D:119:SER:HB2	1.96	0.47
3:E:27:GLU:O	3:E:31:ARG:HB2	2.15	0.47
1:A:203:GLU:N	1:A:203:GLU:OE1	2.44	0.47
2:D:134:ILE:HG22	2:D:136:PRO:HD2	1.96	0.47
4:F:70:ASN:OD1	4:F:70:ASN:N	2.46	0.47
1:C:276:TRP:HB2	1:C:283:PHE:CE1	2.49	0.47
1:C:254:MET:HE1	3:E:13:PHE:HB3	1.96	0.47
3:E:46:LYS:HD2	3:E:48:ARG:NE	2.29	0.47
4:N:15:GLN:O	4:N:19:LYS:HG3	2.15	0.47
1:A:202:PRO:HA	1:A:228:ARG:HD3	1.96	0.47
1:A:412:ASN:O	1:A:416:THR:HG23	2.15	0.47
1:C:137:ILE:HG12	1:C:207:GLU:HG2	1.96	0.47
1:C:244:ARG:HD2	1:C:244:ARG:HA	1.74	0.47
1:C:209:PHE:CE1	1:C:262:VAL:HG21	2.49	0.47
2:B:104:ILE:HG13	2:B:127:LEU:HD13	1.97	0.47
1:C:149:ASN:HB2	1:C:161:VAL:HG22	1.96	0.47
2:B:19:SER:HA	3:J:38:GLY:O	2.15	0.47
1:C:309:VAL:HG13	1:C:314:LEU:HB2	1.96	0.47
3:E:24:GLU:OE2	4:F:47:ARG:NH1	2.46	0.47
4:F:3:ALA:HB1	5:G:19:C:H5	1.78	0.47
3:J:22:THR:HG21	3:J:39:PRO:HB3	1.96	0.47
4:N:71:LEU:O	4:N:74:ILE:HG22	2.14	0.47
1:A:224:LYS:HG3	1:A:276:TRP:CD2	2.49	0.47
1:A:43:ILE:HB	1:A:60:ARG:NH2	2.30	0.47
2:B:27:ILE:HG12	2:B:55:VAL:HG21	1.95	0.47
2:B:62:LEU:HD12	2:B:63:ASP:N	2.30	0.47
1:C:210:ARG:HH11	4:F:42:ARG:HH11	1.62	0.47
1:A:122:GLU:OE2	1:A:191:ARG:NH1	2.46	0.47
1:A:238:VAL:O	1:A:276:TRP:N	2.35	0.47
1:A:355:ALA:O	1:A:358:THR:OG1	2.17	0.47
1:C:111:LYS:O	1:C:115:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:11:ARG:HH11	5:R:24:A:P	2.37	0.47
1:C:389:MET:HE3	1:C:392:LEU:HD11	1.96	0.46
3:J:89:ARG:HB3	4:N:51:ALA:HB1	1.97	0.46
1:A:16:LYS:HD3	1:A:16:LYS:H	1.81	0.46
1:C:41:GLN:HB3	1:C:72:THR:HG21	1.97	0.46
1:C:337:ASN:CG	4:F:24:LEU:HD21	2.36	0.46
1:A:109:THR:O	1:A:112:GLN:HB3	2.15	0.46
1:A:303:HIS:HB3	1:A:334:TRP:CZ3	2.51	0.46
2:B:17:LEU:HD21	2:B:87:ILE:HG12	1.96	0.46
1:A:322:GLY:O	1:A:325:VAL:HG12	2.15	0.46
1:A:363:LEU:HB3	1:A:369:PHE:HZ	1.80	0.46
2:B:109:GLU:O	2:B:112:LYS:HB2	2.15	0.46
1:C:341:VAL:O	1:C:344:LEU:HG	2.15	0.46
1:A:270:ARG:HG3	5:R:13:U:H1'	1.98	0.46
1:C:383:GLU:HG2	1:C:409:ARG:HE	1.81	0.46
3:J:92:LEU:HD23	3:J:92:LEU:H	1.80	0.46
2:B:126:VAL:HG23	5:R:7:U:C4	2.50	0.46
2:B:77:LEU:HG	5:R:8:U:C4	2.51	0.46
4:F:6:ARG:HD2	4:F:6:ARG:HA	1.77	0.46
1:A:339:MET:HE3	4:N:24:LEU:CG	2.46	0.46
2:B:106:GLU:O	2:B:110:LEU:HG	2.15	0.46
1:C:310:GLU:O	1:C:314:LEU:N	2.48	0.46
4:N:70:ASN:HA	4:N:73:ARG:HD2	1.98	0.46
1:A:101:THR:C	1:A:102:PHE:HD1	2.18	0.46
1:A:7:ALA:HA	1:A:10:GLU:HG2	1.98	0.46
1:C:210:ARG:NH1	4:F:42:ARG:HH11	2.14	0.46
1:A:188:PRO:CG	1:C:89:LEU:H	2.28	0.46
1:A:358:THR:O	1:A:362:TYR:HD1	1.99	0.46
1:C:37:LYS:HA	1:C:37:LYS:HD3	1.69	0.46
2:D:8:ARG:HH12	2:D:41:LYS:HD2	1.81	0.46
1:C:250:ALA:HA	5:G:10:A:C6	2.50	0.46
4:N:42:ARG:CZ	4:N:42:ARG:HB2	2.47	0.45
3:E:18:ILE:O	3:E:22:THR:HG22	2.16	0.45
4:F:24:LEU:HD22	4:F:25:LEU:H	1.80	0.45
1:A:63:LEU:O	1:A:74:GLU:HA	2.16	0.45
2:B:112:LYS:HA	2:B:120:HIS:CD2	2.51	0.45
1:C:356:ILE:HD13	1:C:359:PHE:HE2	1.81	0.45
2:D:20:TRP:HD1	2:D:30:VAL:HG21	1.82	0.45
2:D:64:GLY:O	2:D:67:LYS:HG2	2.16	0.45
5:R:26:A:OP1	5:R:26:A:H8	1.99	0.45
1:C:38:LYS:HG3	1:C:39:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ALA:HB1	3:E:15:HIS:NE2	2.31	0.45
1:A:276:TRP:HA	1:A:283:PHE:CE1	2.51	0.45
1:A:281:ALA:O	1:A:285:ILE:HG13	2.17	0.45
3:E:9:ARG:O	3:E:10:LEU:HD23	2.17	0.45
3:J:11:LYS:HE2	3:J:13:PHE:HD2	1.80	0.45
4:N:20:ALA:O	4:N:22:ASN:ND2	2.49	0.45
1:A:339:MET:HB3	4:N:24:LEU:HD23	1.98	0.45
1:C:239:LYS:HD2	1:C:239:LYS:HA	1.53	0.45
2:B:119:SER:HB2	5:R:8:U:C2	2.51	0.45
1:A:252:VAL:HG13	1:A:256:GLY:HA2	1.97	0.45
2:B:124:ASN:O	2:B:127:LEU:HG	2.16	0.45
2:D:103:ALA:O	2:D:107:ALA:CB	2.64	0.45
3:E:10:LEU:CA	3:E:11:LYS:HE2	2.46	0.45
1:A:331:LEU:HD23	4:N:35:ARG:HH22	1.82	0.45
1:A:191:ARG:HD2	1:A:191:ARG:HA	1.75	0.45
1:A:72:THR:HG23	1:A:73:LYS:HG2	1.98	0.45
1:A:399:ASP:OD1	1:A:400:GLU:N	2.50	0.45
2:D:73:LEU:HD22	2:D:75:GLU:HG2	1.98	0.45
2:D:81:GLU:O	2:D:85:LEU:HB2	2.17	0.45
1:A:339:MET:HE3	4:N:24:LEU:HG	1.99	0.45
4:N:64:HIS:O	4:N:68:GLU:HG2	2.17	0.45
4:N:8:ARG:NH2	5:R:25:G:O5'	2.46	0.45
2:B:11:GLU:O	2:B:14:VAL:HB	2.17	0.44
1:C:355:ALA:O	1:C:359:PHE:HD2	1.99	0.44
1:C:391:GLU:N	1:C:391:GLU:OE1	2.42	0.44
2:B:17:LEU:HD12	2:B:18:TYR:N	2.32	0.44
1:C:152:LEU:HD22	1:C:162:ILE:HG13	1.98	0.44
1:C:46:ARG:HB2	1:C:61:ARG:NH2	2.32	0.44
1:C:114:ILE:O	1:C:118:VAL:HG23	2.18	0.44
3:E:86:ALA:HB1	4:F:51:ALA:HB1	1.98	0.44
5:R:20:C:N3	5:R:28:G:N2	2.47	0.44
1:A:373:LEU:HA	1:A:376:GLU:HB3	1.99	0.44
1:C:254:MET:CE	3:E:13:PHE:HB3	2.48	0.44
1:A:255:ARG:HD3	5:R:12:A:H5'	2.00	0.44
1:A:132:GLU:HB3	1:A:133:HIS:ND1	2.33	0.44
1:A:235:LYS:HG3	1:A:327:LEU:HD13	1.98	0.44
1:A:248:VAL:HG12	1:A:273:ILE:HG22	1.99	0.44
2:D:55:VAL:HG23	2:D:62:LEU:HD12	1.99	0.44
2:D:83:ALA:O	2:D:87:ILE:HG22	2.18	0.44
1:A:248:VAL:HG23	5:R:11:C:N4	2.33	0.44
1:A:67:GLU:OE1	1:C:116:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:O	1:C:37:LYS:HG2	2.18	0.44
4:N:42:ARG:NH1	4:N:42:ARG:HB2	2.32	0.44
1:A:104:ARG:HE	1:A:105:ILE:HA	1.82	0.44
1:A:339:MET:CE	1:A:344:LEU:HA	2.47	0.44
1:A:380:THR:HG22	1:A:383:GLU:HB2	2.00	0.44
2:B:111:ALA:CB	2:B:120:HIS:HB3	2.46	0.44
1:C:252:VAL:HG13	1:C:256:GLY:HA2	1.99	0.44
3:E:69:THR:O	3:E:69:THR:OG1	2.35	0.44
3:J:89:ARG:HG2	4:N:51:ALA:HA	2.00	0.44
4:N:45:LYS:HA	4:N:45:LYS:HD2	1.73	0.44
1:A:359:PHE:HB3	1:A:369:PHE:CD1	2.53	0.44
1:A:49:ILE:CG1	1:A:56:PHE:HB3	2.48	0.44
1:C:9:VAL:O	1:C:13:SER:N	2.51	0.44
1:A:223:ILE:O	1:A:223:ILE:HG12	2.18	0.43
1:A:46:ARG:HD3	1:A:46:ARG:HA	1.68	0.43
3:J:12:ALA:HB3	3:J:70:HIS:C	2.39	0.43
3:E:35:GLN:HG3	3:E:77:VAL:HG21	2.00	0.43
4:F:10:ARG:NH2	5:G:20:C:OP2	2.51	0.43
4:N:47:ARG:HD3	4:N:47:ARG:H	1.82	0.43
2:D:116:ALA:HB1	3:E:15:HIS:CE1	2.52	0.43
2:D:28:ALA:O	2:D:31:GLU:HG2	2.18	0.43
4:F:33:VAL:O	4:F:36:PRO:HD2	2.18	0.43
1:A:123:ARG:O	1:A:127:VAL:HG23	2.18	0.43
1:A:65:VAL:HG13	1:A:67:GLU:H	1.82	0.43
1:C:137:ILE:HG12	1:C:207:GLU:CG	2.48	0.43
4:F:6:ARG:O	4:F:10:ARG:HG3	2.18	0.43
1:C:210:ARG:NH1	4:F:42:ARG:HE	2.16	0.43
1:A:307:ILE:O	1:A:339:MET:HG2	2.19	0.43
1:A:308:ALA:HB2	1:A:344:LEU:HG	2.00	0.43
2:B:27:ILE:HD11	2:B:55:VAL:HG11	2.00	0.43
2:B:83:ALA:O	2:B:87:ILE:HG13	2.18	0.43
1:C:117:LYS:HD3	1:C:117:LYS:HA	1.78	0.43
1:A:89:LEU:H	1:C:188:PRO:HG3	1.83	0.43
3:E:64:GLN:H	3:E:64:GLN:NE2	2.16	0.43
4:N:80:ARG:HB2	4:N:82:TRP:HE1	1.82	0.43
1:A:218:GLU:O	1:A:219:GLU:HG2	2.19	0.43
1:C:209:PHE:O	1:C:213:VAL:N	2.43	0.43
1:C:329:SER:OG	4:F:29:SER:OG	2.27	0.43
1:C:84:ASP:HB3	1:C:87:LEU:CD2	2.49	0.43
4:F:61:ALA:O	4:F:65:LYS:HG2	2.19	0.43
4:N:8:ARG:O	4:N:15:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:O	1:A:323:GLN:HG3	2.19	0.43
1:A:188:PRO:HG2	1:C:89:LEU:H	1.83	0.43
3:E:6:ILE:HG21	3:E:101:SER:OG	2.19	0.43
4:F:13:GLU:O	4:F:17:GLN:HG3	2.17	0.43
3:J:70:HIS:C	3:J:71:LEU:HD22	2.39	0.43
1:A:306:ASP:HA	1:A:337:ASN:HB3	2.01	0.43
1:A:398:LEU:O	1:A:402:THR:OG1	2.37	0.43
2:B:120:HIS:CE1	2:B:121:LYS:HE3	2.54	0.43
4:F:35:ARG:O	4:F:38:LEU:HG	2.19	0.43
2:B:104:ILE:CG1	2:B:127:LEU:HD22	2.49	0.43
1:C:146:ASN:HB2	1:C:149:ASN:OD1	2.19	0.43
4:N:24:LEU:CD2	4:N:24:LEU:H	2.08	0.43
1:A:181:GLY:HA2	1:A:204:MET:CE	2.48	0.42
1:A:232:SER:O	1:A:269:GLU:HG3	2.19	0.42
1:A:310:GLU:O	1:A:314:LEU:N	2.52	0.42
1:A:389:MET:HG3	1:A:407:ARG:CZ	2.49	0.42
1:C:145:VAL:HG23	1:C:150:ILE:HG22	2.01	0.42
1:C:409:ARG:O	1:C:413:ALA:N	2.39	0.42
4:N:62:GLU:OE1	4:N:66:GLN:NE2	2.52	0.42
2:B:112:LYS:HG2	2:B:120:HIS:ND1	2.33	0.42
4:N:8:ARG:HH12	5:R:25:G:P	2.43	0.42
1:A:317:ALA:O	1:A:324:ASN:ND2	2.52	0.42
1:A:31:LEU:O	1:A:35:THR:HG23	2.19	0.42
2:B:72:ARG:HE	2:B:72:ARG:CA	2.32	0.42
1:C:342:ASP:N	1:C:342:ASP:OD1	2.50	0.42
3:J:36:VAL:HG21	3:J:75:ASP:C	2.40	0.42
2:B:17:LEU:HD13	2:B:83:ALA:HB1	2.01	0.42
2:B:67:LYS:HE2	2:B:67:LYS:HB3	1.82	0.42
1:C:0:ALA:HA	1:C:3:LYS:HB2	2.00	0.42
3:E:39:PRO:HB3	3:E:74:VAL:HG22	2.00	0.42
2:B:134:ILE:HG22	2:B:136:PRO:HG2	2.01	0.42
1:C:136:GLU:O	1:C:182:VAL:HA	2.20	0.42
2:D:85:LEU:HD13	2:D:85:LEU:HA	1.79	0.42
4:F:15:GLN:HG2	5:G:23:A:O2'	2.20	0.42
1:C:366:ASP:HB2	1:C:369:PHE:CD1	2.54	0.42
2:D:10:ARG:HA	2:D:48:PHE:CE1	2.54	0.42
3:E:31:ARG:NH1	4:F:52:LEU:HG	2.35	0.42
4:F:38:LEU:HD12	4:F:39:SER:HB3	2.02	0.42
1:A:215:GLU:OE2	1:A:215:GLU:N	2.51	0.42
1:A:263:SER:O	1:A:268:GLY:N	2.49	0.42
3:E:46:LYS:HA	3:E:69:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:80:ARG:HB2	4:N:82:TRP:NE1	2.35	0.42
1:C:207:GLU:O	1:C:211:ILE:HG22	2.20	0.42
1:C:76:THR:HG23	1:C:79:ALA:H	1.85	0.42
1:A:145:VAL:HG21	1:A:175:PRO:HD3	2.02	0.42
1:A:244:ARG:HH22	2:B:73:LEU:HD23	1.84	0.42
1:C:234:ALA:O	1:C:271:ILE:HA	2.20	0.42
1:A:154:LEU:HB2	1:A:158:ALA:HB3	2.02	0.42
1:A:224:LYS:HG3	1:A:276:TRP:CD1	2.55	0.42
1:A:284:VAL:HG21	1:A:305:MET:SD	2.60	0.42
4:F:45:LYS:HB2	4:F:49:GLU:HB2	2.02	0.42
1:A:93:VAL:HG12	1:A:94:GLU:N	2.35	0.41
2:B:104:ILE:HD12	2:B:104:ILE:HA	1.82	0.41
1:C:247:PRO:HG2	1:C:275:LEU:HD22	2.02	0.41
3:J:86:ALA:O	3:J:90:LEU:HD13	2.20	0.41
2:B:127:LEU:HD12	5:R:4:U:C4	2.54	0.41
1:C:322:GLY:O	1:C:325:VAL:HG12	2.19	0.41
1:A:102:PHE:N	1:A:102:PHE:HD1	2.18	0.41
1:A:376:GLU:O	1:A:379:SER:N	2.44	0.41
2:B:101:LYS:HZ2	5:R:3:C:H2'	1.85	0.41
4:F:14:LYS:HB3	4:F:14:LYS:HE2	1.91	0.41
3:J:6:ILE:HD11	3:J:79:PRO:HG3	2.02	0.41
1:C:104:ARG:HG2	1:C:105:ILE:N	2.34	0.41
1:C:218:GLU:HB3	1:C:220:VAL:HG23	2.01	0.41
1:A:22:LYS:HE3	1:A:22:LYS:HB3	1.76	0.41
2:B:23:SER:HB2	2:B:25:ASN:ND2	2.35	0.41
1:C:210:ARG:HH12	4:F:42:ARG:HE	1.68	0.41
1:C:224:LYS:HE3	4:F:35:ARG:HH22	1.84	0.41
5:G:11:C:HO2'	5:G:12:A:P	2.43	0.41
1:C:184:TYR:CE1	1:C:196:PHE:HB3	2.56	0.41
1:C:331:LEU:HD12	1:C:331:LEU:HA	1.85	0.41
2:D:68:PRO:HG2	2:D:129:LYS:HD3	2.03	0.41
4:F:70:ASN:HA	4:F:73:ARG:HG2	2.03	0.41
2:B:81:GLU:OE2	5:R:8:U:N3	2.54	0.41
1:A:0:ALA:HB3	1:A:56:PHE:CE1	2.56	0.41
1:A:348:HIS:ND1	1:A:351:GLU:OE1	2.43	0.41
1:A:380:THR:HG23	1:A:383:GLU:H	1.86	0.41
2:B:66:MET:SD	2:B:70:LEU:HD11	2.60	0.41
2:B:95:ARG:HG3	2:B:97:ASP:HB2	2.03	0.41
1:C:229:ASP:OD1	1:C:326:ARG:NH2	2.53	0.41
1:C:64:VAL:HG12	1:C:91:ASP:O	2.21	0.41
1:A:133:HIS:O	1:A:136:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:HG22	5:R:12:A:C8	2.56	0.41
1:A:379:SER:HB3	1:A:383:GLU:HB3	2.03	0.41
1:C:182:VAL:HG11	1:C:203:GLU:HB3	2.03	0.41
1:C:254:MET:HG2	1:C:254:MET:H	1.40	0.41
1:C:359:PHE:O	1:C:363:LEU:HD22	2.20	0.41
3:E:99:GLN:HE21	3:E:100:ILE:H	1.69	0.41
4:F:62:GLU:O	4:F:66:GLN:HB2	2.21	0.41
1:A:159:GLU:C	1:A:194:GLN:HE21	2.25	0.41
1:A:303:HIS:CE1	1:A:334:TRP:CD1	3.09	0.41
2:B:17:LEU:HD12	2:B:18:TYR:H	1.86	0.41
3:J:21:ALA:O	3:J:25:ILE:HG13	2.21	0.41
1:A:102:PHE:N	1:A:102:PHE:CD1	2.89	0.40
1:A:123:ARG:HG3	1:A:124:ALA:N	2.37	0.40
1:A:234:ALA:HB2	1:A:269:GLU:OE1	2.21	0.40
2:D:66:MET:C	2:D:68:PRO:HD2	2.41	0.40
2:D:71:SER:H	5:G:7:U:H3	1.69	0.40
3:J:5:ARG:NH2	3:J:6:ILE:O	2.55	0.40
1:C:410:ALA:O	1:C:413:ALA:HB3	2.21	0.40
4:N:48:VAL:O	4:N:52:LEU:HD22	2.21	0.40
1:C:1:MET:O	1:C:4:GLU:HB3	2.22	0.40
1:C:359:PHE:HB3	1:C:381:LEU:HD13	2.03	0.40
1:C:64:VAL:HA	1:C:75:ILE:O	2.22	0.40
1:C:250:ALA:HA	5:G:10:A:N6	2.37	0.40
4:F:8:ARG:HA	4:F:15:GLN:HE22	1.85	0.40
1:C:4:GLU:OE2	4:F:77:LYS:HE2	2.21	0.40
3:J:12:ALA:HB3	3:J:70:HIS:O	2.21	0.40
1:A:206:ILE:HD12	1:A:223:ILE:HG13	2.04	0.40
2:B:87:ILE:O	2:B:90:TYR:HB3	2.22	0.40
3:E:15:HIS:NE2	5:G:9:A:N1	2.69	0.40
4:N:31:LYS:HG2	4:N:32:PRO:HD2	2.03	0.40
5:R:19:C:H2'	5:R:20:C:H6	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	426/428 (100%)	395 (93%)	30 (7%)	1 (0%)	47 78
1	C	421/428 (98%)	391 (93%)	30 (7%)	0	100 100
2	B	132/141 (94%)	126 (96%)	6 (4%)	0	100 100
2	D	130/141 (92%)	122 (94%)	8 (6%)	0	100 100
3	E	87/108 (81%)	82 (94%)	5 (6%)	0	100 100
3	J	92/108 (85%)	81 (88%)	11 (12%)	0	100 100
4	F	82/89 (92%)	76 (93%)	5 (6%)	1 (1%)	13 44
4	N	83/89 (93%)	76 (92%)	7 (8%)	0	100 100
All	All	1453/1532 (95%)	1349 (93%)	102 (7%)	2 (0%)	51 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	23	PRO
1	A	19	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	357/357 (100%)	313 (88%)	44 (12%)	4 19
1	C	353/357 (99%)	313 (89%)	40 (11%)	6 23
2	B	111/116 (96%)	90 (81%)	21 (19%)	1 6
2	D	110/116 (95%)	97 (88%)	13 (12%)	5 21
3	E	80/93 (86%)	66 (82%)	14 (18%)	2 8
3	J	85/93 (91%)	75 (88%)	10 (12%)	5 21
4	F	74/78 (95%)	66 (89%)	8 (11%)	6 25
4	N	75/78 (96%)	64 (85%)	11 (15%)	3 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1245/1288 (97%)	1084 (87%)	161 (13%)	4 17

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	20	ARG
1	A	35	THR
1	A	46	ARG
1	A	56	PHE
1	A	59	PHE
1	A	72	THR
1	A	75	ILE
1	A	89	LEU
1	A	94	GLU
1	A	102	PHE
1	A	104	ARG
1	A	116	GLN
1	A	119	ARG
1	A	132	GLU
1	A	139	THR
1	A	156	ASN
1	A	170	ARG
1	A	177	ASP
1	A	184	TYR
1	A	186	VAL
1	A	195	LEU
1	A	203	GLU
1	A	207	GLU
1	A	208	LEU
1	A	209	PHE
1	A	223	ILE
1	A	233	ARG
1	A	244	ARG
1	A	254	MET
1	A	255	ARG
1	A	262	VAL
1	A	270	ARG
1	A	275	LEU
1	A	305	MET
1	A	323	GLN
1	A	331	LEU

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Mol	Chain	Res	Type
1	A	347	LYS
1	A	356	ILE
1	A	361	LYS
1	A	381	LEU
1	A	384	LEU
1	A	392	LEU
1	A	408	GLU
2	B	17	LEU
2	B	21	GLN
2	B	26	ASP
2	B	29	ASP
2	B	32	TYR
2	B	41	LYS
2	B	65	LEU
2	B	66	MET
2	B	72	ARG
2	B	74	LEU
2	B	75	GLU
2	B	79	GLN
2	B	86	ARG
2	B	89	LEU
2	B	100	TYR
2	B	101	LYS
2	B	124	ASN
2	B	126	VAL
2	B	127	LEU
2	B	134	ILE
2	B	137	ASN
3	J	11	LYS
3	J	13	PHE
3	J	22	THR
3	J	27	GLU
3	J	37	ARG
3	J	53	ILE
3	J	57	VAL
3	J	63	ASP
3	J	66	GLU
3	J	90	LEU
4	N	11	ARG
4	N	24	LEU
4	N	31	LYS
4	N	34	ASN

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Mol	Chain	Res	Type
4	N	37	ILE
4	N	40	LEU
4	N	47	ARG
4	N	48	VAL
4	N	52	LEU
4	N	58	THR
4	N	66	GLN
1	C	1	MET
1	C	12	VAL
1	C	40	GLU
1	C	57	ASP
1	C	73	LYS
1	C	86	SER
1	C	102	PHE
1	C	104	ARG
1	C	113	VAL
1	C	142	VAL
1	C	161	VAL
1	C	168	LEU
1	C	191	ARG
1	C	209	PHE
1	C	215	GLU
1	C	228	ARG
1	C	239	LYS
1	C	240	THR
1	C	254	MET
1	C	255	ARG
1	C	272	ASP
1	C	276	TRP
1	C	278	ASP
1	C	279	ASN
1	C	340	THR
1	C	342	ASP
1	C	349	GLN
1	C	359	PHE
1	C	363	LEU
1	C	366	ASP
1	C	371	THR
1	C	378	PHE
1	C	381	LEU
1	C	384	LEU
1	C	387	VAL

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Mol	Chain	Res	Type
1	C	389	MET
1	C	390	LYS
1	C	392	LEU
1	C	406	LEU
1	C	409	ARG
2	D	6	ARG
2	D	32	TYR
2	D	69	TYR
2	D	73	LEU
2	D	80	VAL
2	D	85	LEU
2	D	101	LYS
2	D	105	ASN
2	D	106	GLU
2	D	124	ASN
2	D	128	ASP
2	D	129	LYS
2	D	133	VAL
3	E	2	GLN
3	E	9	ARG
3	E	11	LYS
3	E	17	LEU
3	E	32	THR
3	E	35	GLN
3	E	40	ILE
3	E	45	ARG
3	E	64	GLN
3	E	68	ARG
3	E	77	VAL
3	E	92	LEU
3	E	97	ASP
3	E	99	GLN
4	F	8	ARG
4	F	24	LEU
4	F	26	VAL
4	F	35	ARG
4	F	45	LYS
4	F	55	ILE
4	F	70	ASN
4	F	77	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	14	ASN
1	A	156	ASN
1	A	286	ASN
2	B	120	HIS
1	C	133	HIS
1	C	324	ASN
1	C	421	GLN
4	F	22	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	G	26/30 (86%)	10 (38%)	0
5	R	29/30 (96%)	15 (51%)	5 (17%)
All	All	55/60 (91%)	25 (45%)	5 (9%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	4	U
5	R	5	C
5	R	6	U
5	R	7	U
5	R	8	U
5	R	9	A
5	R	10	A
5	R	11	C
5	R	12	A
5	R	14	U
5	R	15	A
5	R	17	G
5	R	24	A
5	R	25	G
5	R	29	G
5	G	6	U
5	G	7	U
5	G	8	U
5	G	10	A
5	G	11	C
5	G	12	A
5	G	14	U

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Mol	Chain	Res	Type
5	G	15	A
5	G	17	G
5	G	25	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	3	C
5	R	9	A
5	R	10	A
5	R	11	C
5	R	14	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

There are no ligands in this entry.

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	A	428/428 (100%)	0.16	12 (2%) 53 55	52, 111, 223, 267	0
1	C	423/428 (98%)	0.20	15 (3%) 44 46	54, 110, 252, 312	0
2	B	134/141 (95%)	0.30	8 (5%) 21 24	108, 183, 227, 237	0
2	D	132/141 (93%)	0.30	9 (6%) 17 20	123, 172, 211, 233	0
3	E	91/108 (84%)	0.47	6 (6%) 18 21	81, 136, 176, 207	0
3	J	96/108 (88%)	0.61	7 (7%) 15 17	92, 136, 207, 226	0
4	F	84/89 (94%)	0.25	8 (9%) 8 10	86, 158, 221, 253	0
4	N	85/89 (95%)	0.36	9 (10%) 6 7	69, 146, 236, 282	0
5	G	27/30 (90%)	-0.08	0 100 100	104, 141, 174, 180	0
5	R	29/30 (96%)	-0.09	0 100 100	91, 123, 239, 243	0
All	All	1529/1592 (96%)	0.25	74 (4%) 30 33	52, 135, 229, 312	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	PHE	6.6
1	C	305	MET	5.3
2	D	130	ALA	4.5
1	A	406	LEU	4.4
1	A	308	ALA	4.1
2	B	52	LEU	4.0
4	N	82	TRP	3.9
2	D	104	ILE	3.8
3	J	63	ASP	3.7
2	B	88	ALA	3.6
1	A	395	ILE	3.5
4	F	17	GLN	3.5
1	A	237	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
4	N	79	GLN	3.4
4	N	33	VAL	3.3
4	F	36	PRO	3.3
1	A	307	ILE	3.2
2	B	91	GLU	3.1
4	F	63	TYR	3.0
1	A	306	ASP	2.9
2	D	63	ASP	2.9
4	N	80	ARG	2.9
1	C	-1	GLY	2.9
4	F	14	LYS	2.8
4	F	33	VAL	2.8
1	C	240	THR	2.7
1	C	332	SER	2.7
2	D	90	TYR	2.7
4	F	30	ALA	2.6
3	J	79	PRO	2.6
1	A	417	ILE	2.6
1	C	245	ILE	2.6
4	N	81	THR	2.6
1	C	408	GLU	2.5
3	J	81	GLU	2.5
4	N	72	GLN	2.5
1	C	389	MET	2.5
4	N	44	PRO	2.5
3	E	5	ARG	2.4
1	C	193	ALA	2.4
3	E	26	VAL	2.4
1	C	381	LEU	2.4
1	A	292	ASP	2.4
4	N	32	PRO	2.4
3	J	28	THR	2.3
2	D	33	GLN	2.3
2	B	86	ARG	2.3
3	E	22	THR	2.3
1	C	363	LEU	2.3
3	J	95	GLY	2.3
3	J	50	THR	2.3
2	D	38	GLN	2.2
4	F	72	GLN	2.2
1	C	346	ALA	2.2
1	C	307	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	J	101	SER	2.1
4	N	78	ASN	2.1
1	A	15	GLU	2.1
2	D	85	LEU	2.1
2	B	4	ALA	2.1
2	B	8	ARG	2.1
2	B	131	ALA	2.1
1	A	227	ALA	2.1
1	C	242	ASP	2.1
1	A	56	PHE	2.1
1	A	235	LYS	2.1
3	E	10	LEU	2.1
3	E	69	THR	2.0
2	D	91	GLU	2.0
3	E	48	ARG	2.0
1	C	357	ASP	2.0
2	D	84	VAL	2.0
1	C	369	PHE	2.0
4	F	78	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.