



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:56 PM UTC

PDB ID : 7OXQ / pdb_00007oxq
Title : Crystal structure of HIV-1 reverse transcriptase with a double stranded DNA in complex with fragment 048 at the transient P-pocket.
Authors : Martinez, S.E.; Singh, A.K.; Das, K.
Deposited on : 2021-06-22
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

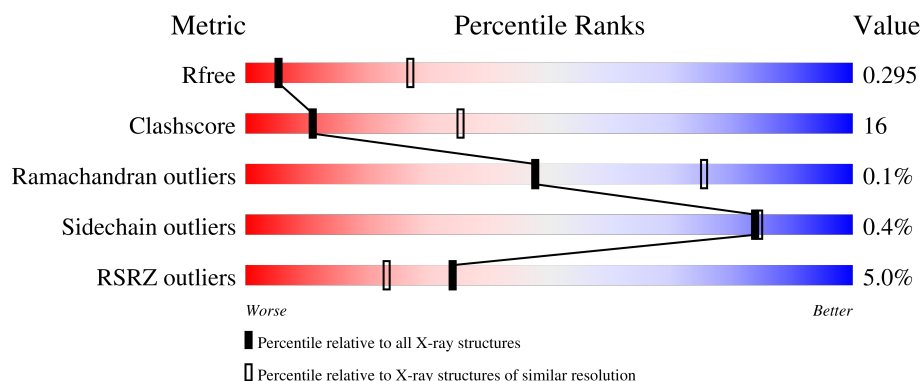
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	556	6% 67% 33%
1	C	556	6% 62% 37% .
2	B	444	3% 64% 30% 6%
2	D	444	4% 59% 32% . 9%
3	E	28	46% 32% 21%

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Mol	Chain	Length	Quality of chain
3	T	28	 61% 21% 18%
4	F	21	 71% 24% 5%
4	P	21	 67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17577 atoms, of which 12 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4504	2913	749	834	8			
1	C	551	Total	C	N	O	S	0	0	0
			4486	2902	747	829	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	63	CYS	ILE	conflict	UNP P03366
A	280	SER	CYS	conflict	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	63	CYS	ILE	conflict	UNP P03366
C	280	SER	CYS	conflict	UNP P03366

- Molecule 2 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	0	0
			3431	2228	572	625	6			
2	D	406	Total	C	N	O	S	0	0	0
			3349	2180	552	611	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P03366
B	-14	ALA	-	expression tag	UNP P03366
B	-13	HIS	-	expression tag	UNP P03366
B	-12	HIS	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P03366
B	-10	HIS	-	expression tag	UNP P03366
B	-9	HIS	-	expression tag	UNP P03366
B	-8	HIS	-	expression tag	UNP P03366
B	-7	ALA	-	expression tag	UNP P03366
B	-6	LEU	-	expression tag	UNP P03366
B	-5	GLU	-	expression tag	UNP P03366
B	-4	VAL	-	expression tag	UNP P03366
B	-3	LEU	-	expression tag	UNP P03366
B	-2	PHE	-	expression tag	UNP P03366
B	-1	GLN	-	expression tag	UNP P03366
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	-15	MET	-	initiating methionine	UNP P03366
D	-14	ALA	-	expression tag	UNP P03366
D	-13	HIS	-	expression tag	UNP P03366
D	-12	HIS	-	expression tag	UNP P03366
D	-11	HIS	-	expression tag	UNP P03366
D	-10	HIS	-	expression tag	UNP P03366
D	-9	HIS	-	expression tag	UNP P03366
D	-8	HIS	-	expression tag	UNP P03366
D	-7	ALA	-	expression tag	UNP P03366
D	-6	LEU	-	expression tag	UNP P03366
D	-5	GLU	-	expression tag	UNP P03366
D	-4	VAL	-	expression tag	UNP P03366
D	-3	LEU	-	expression tag	UNP P03366
D	-2	PHE	-	expression tag	UNP P03366
D	-1	GLN	-	expression tag	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	23	Total	C	N	O	P	0	0	0
			474	223	92	136	23			
3	E	22	Total	C	N	O	P	0	0	0
			454	213	90	129	22			

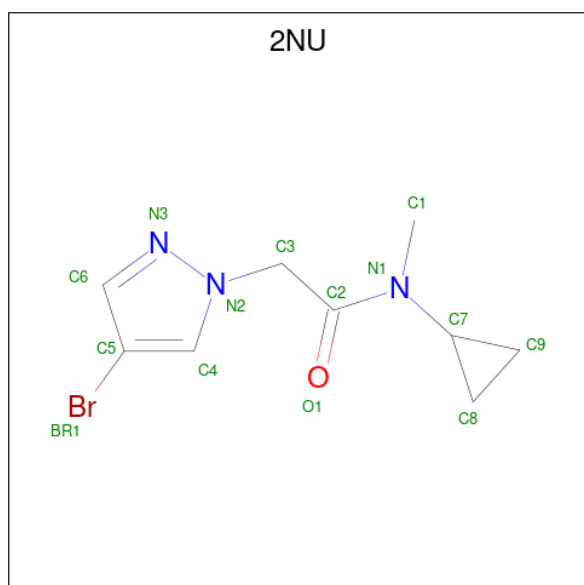
- Molecule 4 is a DNA chain called DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	21	Total	C	N	O	P	0	0	0
			425	202	77	126	20			
4	F	20	Total	C	N	O	P	0	0	0
			407	192	72	123	20			

- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cd	0	0
			3	3		
5	B	3	Total	Cd	0	0
			3	3		
5	T	2	Total	Cd	0	0
			2	2		
5	P	1	Total	Cd	0	0
			1	1		
5	C	3	Total	Cd	0	0
			3	3		
5	D	6	Total	Cd	0	0
			6	6		
5	E	2	Total	Cd	0	0
			2	2		
5	F	1	Total	Cd	0	0
			1	1		

- Molecule 6 is 2-(4-bromanylpyrazol-1-yl)- {N}-cyclopropyl- {N}-methyl-ethanamide (CCD ID: 2NU) (formula: C₉H₁₂BrN₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	Br	C	H	N	O	0	0
			26	1	9	12	3	1		

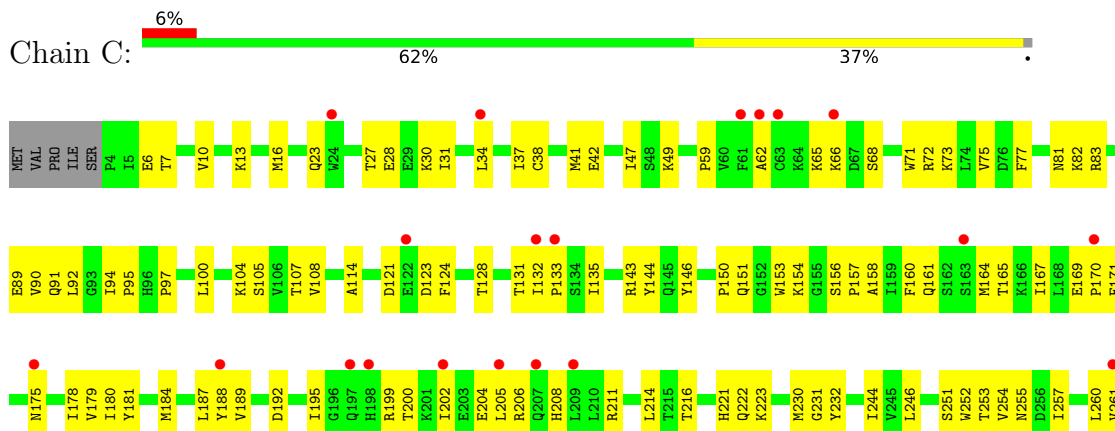
3 Residue-property plots

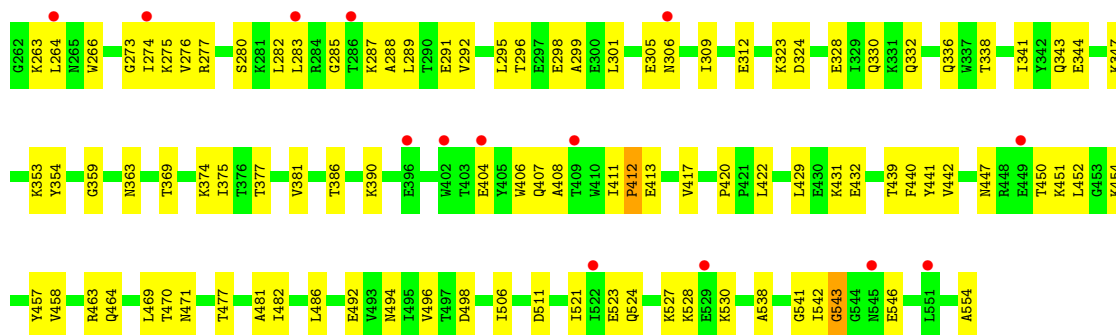
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Reverse transcriptase/ribonuclease H

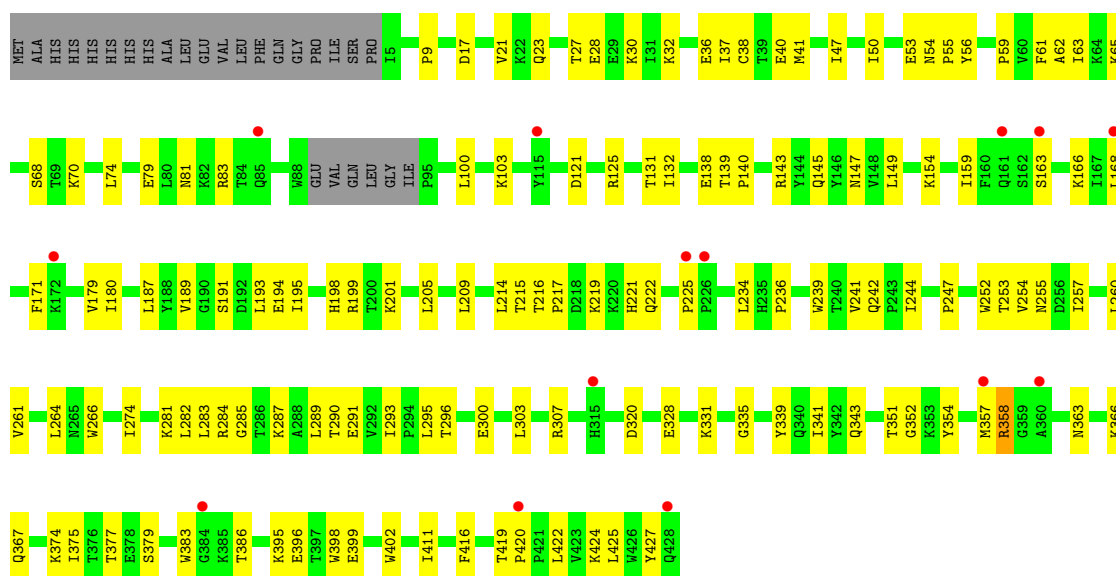


• Molecule 1: Reverse transcriptase/ribonuclease H

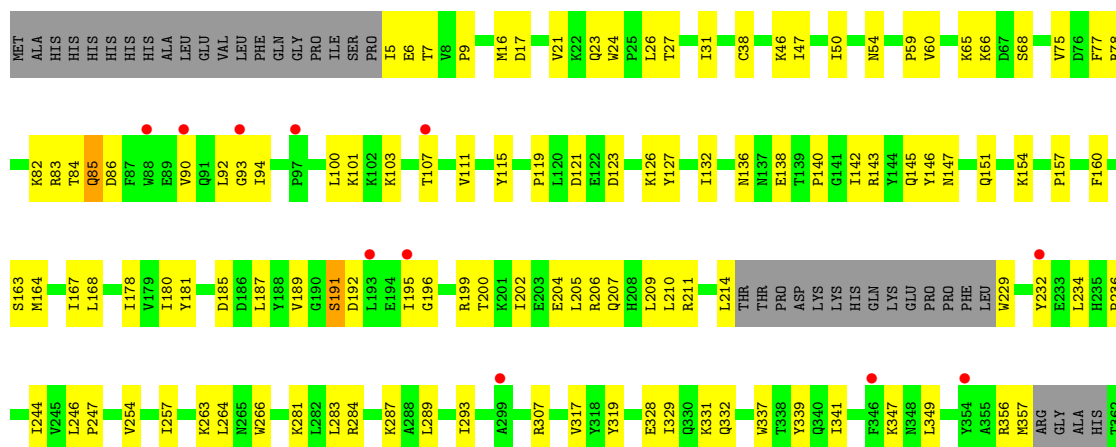




• Molecule 2: Gag-Pol polyprotein



• Molecule 2: Gag-Pol polyprotein





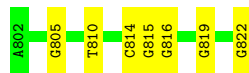
- Molecule 3: DNA (28-MER)



- Molecule 3: DNA (28-MER)



- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3')



- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	309.56Å 61.90Å 168.78Å 90.00° 104.55° 90.00°	Depositor
Resolution (Å)	81.68 – 3.30 81.68 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.8 (81.68-3.30) 93.8 (81.68-3.30)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.262 , 0.296 0.262 , 0.295	Depositor DCC
R_{free} test set	2250 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	17577	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2NU, CD

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	0.25	0/4622	0.49	0/6283
1	C	0.25	0/4603	0.55	1/6252 (0.0%)
2	B	0.37	2/3530 (0.1%)	0.61	7/4797 (0.1%)
2	D	0.36	1/3442 (0.0%)	0.59	4/4674 (0.1%)
3	E	0.46	0/510	0.64	0/785
3	T	0.37	0/532	0.56	0/819
4	F	0.48	0/454	0.74	0/698
4	P	0.46	0/475	0.70	0/731
All	All	0.32	3/18168 (0.0%)	0.57	12/25039 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	154	LYS	CA-C	-7.57	1.43	1.52
2	B	424	LYS	CA-C	-5.30	1.45	1.52
2	B	398	TRP	CA-C	-5.17	1.46	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	424	LYS	N-CA-C	-11.98	97.98	112.59
2	B	357	MET	N-CA-C	9.45	125.69	111.04
2	B	358	ARG	N-CA-CB	6.71	123.37	111.69
2	D	247	PRO	CA-C-O	-6.27	113.78	121.31
2	B	386	THR	CA-C-N	-5.92	114.46	120.85
2	B	386	THR	C-N-CA	-5.92	114.46	120.85
2	D	90	VAL	N-CA-C	5.66	117.54	112.17
2	B	357	MET	CB-CA-C	-5.42	102.78	111.39
2	D	93	GLY	N-CA-C	5.39	125.96	113.18
2	B	358	ARG	N-CA-C	-5.30	101.24	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	412	PRO	CB-CA-C	-5.20	102.34	110.96
2	D	85	GLN	N-CA-C	5.01	117.16	110.35

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	A	4504	0	4543	170	0
1	C	4486	0	4538	197	1
2	B	3431	0	3431	104	1
2	D	3349	0	3370	109	1
3	E	454	0	245	6	0
3	T	474	0	257	5	1
4	F	407	0	225	8	0
4	P	425	0	237	10	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	6	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	P	1	0	0	0	0
5	T	2	0	0	0	0
6	C	14	12	0	2	0
All	All	17565	12	16846	564	2

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 16.

All (564) 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:C:131:THR:HG22	1:C:143:ARG:HG2	1.18	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:HE1	1:A:83:ARG:HA	1.40	1.03
1:C:202:ILE:HG21	1:C:223:LYS:HZ2	1.18	1.02
2:B:281:LYS:HG2	2:B:284:ARG:CZ	1.89	1.02
1:C:202:ILE:HG21	1:C:223:LYS:NZ	1.75	1.01
2:B:281:LYS:HG2	2:B:284:ARG:NH1	1.80	0.96
1:A:84:THR:HB	1:A:154:LYS:HE2	1.46	0.96
2:B:281:LYS:HG2	2:B:284:ARG:NH2	1.81	0.95
2:D:24:TRP:CH2	2:D:403:THR:HG21	2.02	0.94
1:A:13:LYS:HB2	1:A:16:MET:HE2	1.50	0.93
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.54	0.88
1:C:199:ARG:HG2	1:C:223:LYS:HE2	1.56	0.88
1:A:235:HIS:CE1	1:C:312:GLU:HG3	2.11	0.85
1:C:275:LYS:HE2	1:C:332:GLN:OE1	1.78	0.84
1:C:23:GLN:HG2	1:C:133:PRO:HD3	1.59	0.83
1:A:65:LYS:HG2	1:A:72:ARG:HB2	1.61	0.82
1:A:23:GLN:HG2	1:A:133:PRO:HG3	1.61	0.81
1:A:235:HIS:CD2	1:A:236:PRO:HD2	2.15	0.81
1:C:246:LEU:HD23	1:C:260:LEU:HD11	1.64	0.79
2:D:5:ILE:HG22	2:D:6:GLU:H	1.47	0.79
1:C:104:LYS:HD2	1:C:192:ASP:O	1.80	0.79
2:D:107:THR:OG1	2:D:202:ILE:HD11	1.83	0.79
2:D:195:ILE:O	2:D:199:ARG:HG3	1.82	0.79
1:A:324:ASP:O	1:A:343:GLN:HG2	1.83	0.78
2:D:16:MET:HE2	2:D:83:ARG:HG2	1.64	0.78
2:D:365:VAL:O	2:D:369:THR:HG23	1.83	0.77
1:C:180:ILE:CD1	1:C:189:VAL:HG13	2.14	0.77
1:C:231:GLY:N	4:F:822:DG:H5'	2.00	0.77
1:A:402:TRP:O	2:B:331:LYS:NZ	2.17	0.76
1:A:101:LYS:HE2	1:A:321:PRO:CG	2.17	0.75
2:B:219:LYS:O	2:B:222:GLN:NE2	2.19	0.75
2:D:369:THR:HG22	2:D:398:TRP:CH2	2.21	0.75
1:A:110:ASP:HB3	1:A:220:LYS:HB3	1.68	0.75
1:A:26:LEU:HD11	1:A:60:VAL:O	1.86	0.74
1:C:47:ILE:CG2	1:C:144:TYR:HB3	2.18	0.74
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.69	0.74
1:C:77:PHE:O	1:C:81:ASN:ND2	2.20	0.73
2:D:66:LYS:HG3	2:D:407:GLN:OE1	1.88	0.73
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.24	0.73
1:C:107:THR:HG23	1:C:223:LYS:HD3	1.70	0.73
1:A:13:LYS:HB2	1:A:16:MET:CE	2.19	0.73
1:C:206:ARG:NH2	1:C:216:THR:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.54	0.72
1:A:30:LYS:NZ	3:T:705:DT:O4	2.22	0.72
1:C:180:ILE:HD11	1:C:189:VAL:HG13	1.72	0.72
2:B:55:PRO:HG2	2:B:56:TYR:CE1	2.25	0.71
1:C:91:GLN:HB2	1:C:161:GLN:HE22	1.55	0.71
1:C:10:VAL:HG12	1:C:124:PHE:CD1	2.25	0.71
1:C:94:ILE:CG2	1:C:230:MET:HE2	2.21	0.71
1:C:246:LEU:HD23	1:C:260:LEU:CD1	2.20	0.71
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.70	0.71
1:C:131:THR:CG2	1:C:143:ARG:HG2	2.10	0.71
1:A:54:ASN:O	1:A:143:ARG:NH1	2.23	0.70
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.73	0.70
1:C:230:MET:HA	4:F:822:DG:H4'	1.74	0.70
1:A:160:PHE:CZ	1:A:164:MET:HE2	2.26	0.70
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.73	0.70
1:C:199:ARG:HG2	1:C:223:LYS:CE	2.21	0.69
1:C:81:ASN:OD1	1:C:154:LYS:N	2.26	0.69
2:B:100:LEU:HB2	2:B:179:VAL:HG11	1.75	0.69
1:C:408:ALA:O	2:D:393:ILE:HG13	1.92	0.69
1:C:231:GLY:HA3	4:F:822:DG:OP1	1.92	0.69
1:A:274:ILE:HD12	1:A:309:ILE:HD11	1.74	0.68
1:A:30:LYS:HE2	1:A:62:ALA:O	1.94	0.68
1:A:23:GLN:HG2	1:A:133:PRO:CG	2.24	0.68
1:C:298:GLU:N	1:C:298:GLU:OE1	2.27	0.68
2:D:27:THR:O	2:D:31:ILE:HG13	1.94	0.68
1:A:65:LYS:CG	1:A:72:ARG:HB2	2.24	0.68
1:A:0:VAL:CB	1:A:215:THR:HG23	2.24	0.67
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.76	0.67
2:B:30:LYS:NZ	2:B:62:ALA:O	2.27	0.67
1:A:16:MET:CE	1:A:83:ARG:HA	2.22	0.67
2:B:247:PRO:O	2:B:307:ARG:NH2	2.28	0.67
1:C:38:CYS:SG	1:C:132:ILE:HD11	2.35	0.67
1:C:161:GLN:OE1	1:C:184:MET:HE1	1.95	0.67
3:E:706:DC:H2'	3:E:707:DG:C8	2.30	0.67
1:A:23:GLN:HG2	1:A:133:PRO:HD3	1.78	0.66
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.76	0.66
2:B:281:LYS:CG	2:B:284:ARG:NH2	2.58	0.66
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.78	0.66
2:D:151:GLN:HB3	2:D:185:ASP:OD2	1.95	0.66
1:A:23:GLN:HG2	1:A:133:PRO:CD	2.26	0.66
1:A:500:GLN:HG2	2:B:422:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:HIS:NE2	1:C:312:GLU:HG3	2.11	0.65
2:D:16:MET:CE	2:D:83:ARG:HG2	2.26	0.65
1:C:107:THR:CG2	1:C:223:LYS:HD3	2.25	0.65
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.79	0.65
2:D:23:GLN:NE2	2:D:60:VAL:O	2.26	0.65
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.26	0.65
2:B:191:SER:OG	2:B:198:HIS:ND1	2.22	0.65
1:C:13:LYS:HD2	1:C:82:LYS:O	1.97	0.65
2:D:244:ILE:HD11	2:D:426:TRP:CZ3	2.32	0.65
2:D:17:ASP:O	2:D:83:ARG:HD3	1.97	0.64
1:C:94:ILE:HG23	1:C:230:MET:HE2	1.80	0.64
2:B:281:LYS:HG2	2:B:284:ARG:HH12	1.60	0.64
1:C:288:ALA:HB3	1:C:291:GLU:HB2	1.79	0.64
2:D:82:LYS:HE2	2:D:413:GLU:OE2	1.96	0.64
2:D:257:ILE:HG22	2:D:283:LEU:HD11	1.79	0.64
1:C:65:LYS:HG2	1:C:66:LYS:H	1.62	0.64
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.33	0.64
1:A:448:ARG:HH12	4:P:805:DG:H21	1.46	0.64
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.38	0.64
2:D:281:LYS:HB3	2:D:284:ARG:HH12	1.63	0.64
1:C:175:ASN:HB3	1:C:178:ILE:HG12	1.80	0.64
1:A:60:VAL:HG11	1:A:132:ILE:HD13	1.81	0.63
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.33	0.63
1:A:390:LYS:HB3	1:A:417:VAL:HG11	1.78	0.63
1:C:199:ARG:CG	1:C:223:LYS:HE2	2.29	0.63
1:C:254:VAL:CG1	1:C:289:LEU:HA	2.29	0.63
1:A:75:VAL:HB	1:A:77:PHE:CE2	2.34	0.63
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.80	0.63
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.80	0.63
2:D:207:GLN:HA	2:D:210:LEU:CB	2.29	0.62
2:D:207:GLN:HA	2:D:210:LEU:HB2	1.80	0.62
1:C:16:MET:HE2	1:C:83:ARG:HG2	1.81	0.62
2:B:281:LYS:HG2	2:B:284:ARG:HH22	1.61	0.62
1:C:276:VAL:HG22	1:C:353:LYS:HE2	1.82	0.62
1:C:253:THR:HG23	1:C:291:GLU:O	2.00	0.62
2:D:101:LYS:O	2:D:236:PRO:HB2	1.99	0.62
1:A:24:TRP:HH2	1:A:76:ASP:OD2	1.83	0.61
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.82	0.61
2:B:17:ASP:O	2:B:83:ARG:HD3	2.00	0.61
1:C:323:LYS:HE3	1:C:344:GLU:HG2	1.82	0.61
2:D:281:LYS:CB	2:D:284:ARG:HH12	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:CG	1:A:133:PRO:HG3	2.31	0.61
2:D:287:LYS:HD3	2:D:293:ILE:HD11	1.83	0.61
2:B:68:SER:OG	2:B:70:LYS:HD2	2.00	0.61
1:C:27:THR:O	1:C:31:ILE:HG13	2.00	0.60
2:D:5:ILE:HG22	2:D:6:GLU:N	2.14	0.60
1:C:27:THR:HG22	1:C:30:LYS:HD2	1.83	0.60
2:D:372:VAL:HG13	2:D:389:PHE:CZ	2.35	0.60
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.83	0.60
1:A:160:PHE:CE1	1:A:164:MET:HE2	2.36	0.60
1:A:185:ASP:OD2	4:P:822:DG:H5'	2.00	0.60
2:B:195:ILE:O	2:B:199:ARG:HG3	2.01	0.60
2:B:205:LEU:O	2:B:209:LEU:HG	2.02	0.60
2:B:65:LYS:HD2	2:B:70:LYS:HB2	1.82	0.60
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.83	0.60
1:A:10:VAL:C	1:A:11:LYS:HD2	2.25	0.60
1:A:543:GLY:HA2	2:B:283:LEU:O	2.02	0.59
1:C:89:GLU:HG3	1:C:158:ALA:HB2	1.83	0.59
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.02	0.59
1:C:42:GLU:OE2	1:C:49:LYS:HE3	2.02	0.59
1:A:77:PHE:O	1:A:81:ASN:ND2	2.34	0.59
2:D:363:ASN:O	2:D:367:GLN:HG3	2.02	0.59
1:A:281:LYS:HG3	1:A:284:ARG:HE	1.67	0.59
2:B:354:TYR:CE2	2:B:374:LYS:HB3	2.38	0.59
2:D:196:GLY:O	2:D:200:THR:HG23	2.02	0.59
1:A:172:LYS:HE2	1:A:180:ILE:HB	1.85	0.58
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.84	0.58
2:D:357:MET:HE1	2:D:371:ALA:HB2	1.84	0.58
3:E:709:DC:H2'	3:E:710:DG:C8	2.38	0.58
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.84	0.58
6:C:601:2NU:C7	4:F:822:DG:H2'	2.33	0.58
2:B:37:ILE:O	2:B:41:MET:HG3	2.04	0.58
1:C:16:MET:CE	1:C:83:ARG:HG2	2.33	0.58
1:C:498:ASP:HB2	1:C:538:ALA:HB2	1.84	0.58
1:C:282:LEU:HD21	1:C:299:ALA:HB2	1.84	0.58
2:D:103:LYS:HD2	2:D:191:SER:HA	1.85	0.58
2:D:206:ARG:O	2:D:210:LEU:HB2	2.03	0.58
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.85	0.58
1:C:27:THR:HG23	1:C:30:LYS:H	1.69	0.58
2:D:107:THR:HG21	2:D:202:ILE:HD13	1.85	0.58
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.04	0.57
1:C:91:GLN:HB2	1:C:161:GLN:NE2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:GLU:HG2	1:C:330:GLN:NE2	2.20	0.57
2:D:9:PRO:HA	2:D:121:ASP:OD2	2.05	0.57
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.87	0.57
1:C:359:GLY:HA2	4:F:812:DT:OP2	2.05	0.56
2:D:317:VAL:HG22	2:D:347:LYS:HD3	1.87	0.56
1:C:208:HIS:HA	1:C:211:ARG:NE	2.20	0.56
2:D:254:VAL:HG21	2:D:287:LYS:HB2	1.86	0.56
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.86	0.56
1:A:167:ILE:HD12	1:A:214:LEU:HD11	1.87	0.56
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.87	0.56
1:C:328:GLU:HG2	1:C:330:GLN:HE21	1.70	0.56
2:D:390:LYS:HE2	2:D:415:GLU:OE2	2.06	0.56
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.41	0.56
1:A:33:ALA:O	1:A:37:ILE:HG12	2.05	0.56
1:A:274:ILE:HD12	1:A:309:ILE:CD1	2.35	0.56
1:C:406:TRP:CD1	1:C:407:GLN:HG2	2.41	0.56
3:E:713:DC:H2'	3:E:714:DG:C8	2.41	0.56
1:A:235:HIS:NE2	1:C:312:GLU:CG	2.69	0.55
2:B:171:PHE:CD2	2:B:205:LEU:HD13	2.40	0.55
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.06	0.55
2:D:369:THR:HG22	2:D:398:TRP:CZ3	2.41	0.55
1:C:202:ILE:HG21	1:C:223:LYS:HZ1	1.71	0.55
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.06	0.54
2:B:247:PRO:HG2	2:B:252:TRP:CH2	2.42	0.54
1:C:280:SER:O	1:C:283:LEU:HG	2.07	0.54
1:A:257:ILE:HG22	1:A:283:LEU:HD21	1.88	0.54
1:A:266:TRP:CE2	4:P:819:DG:H4'	2.43	0.54
2:B:281:LYS:CD	2:B:284:ARG:HH22	2.21	0.54
2:B:328:GLU:O	2:B:339:TYR:HA	2.08	0.54
1:C:23:GLN:CG	1:C:133:PRO:HD3	2.33	0.54
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.88	0.54
2:D:206:ARG:O	2:D:210:LEU:N	2.39	0.54
1:C:181:TYR:O	1:C:187:LEU:HD12	2.07	0.54
2:D:232:TYR:CD2	2:D:234:LEU:HD21	2.41	0.54
1:C:420:PRO:HA	1:C:422:LEU:HD12	1.89	0.54
2:D:163:SER:O	2:D:167:ILE:HG13	2.07	0.54
2:B:281:LYS:CG	2:B:284:ARG:HH22	2.20	0.54
2:D:103:LYS:HD2	2:D:191:SER:CA	2.37	0.54
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.38	0.54
1:C:181:TYR:CD2	2:D:138:GLU:HA	2.43	0.54
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:HA	1:A:422:LEU:HD12	1.90	0.53
1:C:251:SER:O	1:C:252:TRP:CD1	2.61	0.53
2:D:263:LYS:HA	2:D:425:LEU:HD22	1.90	0.53
1:A:235:HIS:CE1	1:C:312:GLU:CG	2.87	0.53
1:C:202:ILE:O	1:C:206:ARG:HG3	2.08	0.53
2:D:395:LYS:HG3	2:D:416:PHE:CE2	2.43	0.53
4:P:814:DC:H2''	4:P:815:DG:C8	2.44	0.53
1:C:65:LYS:HG2	1:C:66:LYS:N	2.23	0.53
1:C:254:VAL:HG11	1:C:289:LEU:HA	1.89	0.53
1:A:308:GLU:O	1:A:311:LYS:HG2	2.08	0.53
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.08	0.53
1:A:167:ILE:CD1	1:A:214:LEU:HD11	2.39	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.91	0.53
1:C:282:LEU:HD22	1:C:296:THR:HG23	1.91	0.53
2:D:164:MET:HE2	2:D:187:LEU:HD13	1.91	0.53
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.44	0.53
1:A:257:ILE:CG2	1:A:283:LEU:HD21	2.38	0.53
2:B:234:LEU:HD11	2:B:377:THR:CG2	2.39	0.53
2:B:216:THR:HG23	2:B:217:PRO:HD2	1.91	0.52
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.92	0.52
1:C:277:ARG:HD2	1:C:336:GLN:CD	2.34	0.52
1:A:332:GLN:HG3	1:A:333:GLY:H	1.74	0.52
2:B:295:LEU:HB2	2:B:300:GLU:OE2	2.10	0.52
1:C:541:GLY:HA2	1:C:546:GLU:OE1	2.09	0.52
1:A:266:TRP:CZ2	4:P:819:DG:H4'	2.43	0.52
1:C:451:LYS:HB3	1:C:471:ASN:HA	1.92	0.52
1:C:202:ILE:HG13	1:C:223:LYS:HE3	1.92	0.52
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.09	0.52
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.45	0.52
1:C:94:ILE:HD11	3:E:707:DG:H21	1.74	0.52
1:C:150:PRO:HG2	1:C:153:TRP:HB2	1.91	0.52
2:B:282:LEU:HB3	2:B:293:ILE:CG2	2.40	0.52
2:D:372:VAL:HG13	2:D:389:PHE:CE2	2.45	0.52
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.93	0.51
1:A:358:ARG:HD2	1:A:370:GLU:CD	2.35	0.51
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.92	0.51
1:C:264:LEU:CD2	1:C:306:ASN:HB3	2.41	0.51
2:D:418:ASN:OD1	2:D:418:ASN:N	2.42	0.51
2:B:163:SER:O	2:B:166:LYS:HG2	2.11	0.51
2:D:317:VAL:HG12	2:D:349:LEU:HD23	1.92	0.51
3:T:704:DA:H2'	3:T:705:DT:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:VAL:HG12	1:C:289:LEU:O	2.10	0.51
1:A:59:PRO:O	1:A:75:VAL:HG13	2.11	0.51
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.11	0.51
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.93	0.51
1:C:100:LEU:CD2	1:C:181:TYR:CE1	2.93	0.51
1:C:386:THR:HG21	2:D:401:TRP:HH2	1.75	0.51
2:D:420:PRO:HG2	2:D:421:PRO:HD3	1.93	0.51
1:C:169:GLU:N	1:C:170:PRO:HD2	2.26	0.51
1:C:244:ILE:HG23	1:C:263:LYS:HD3	1.93	0.51
2:D:78:ARG:HD3	2:D:411:ILE:HG22	1.92	0.51
2:D:205:LEU:O	2:D:209:LEU:HG	2.10	0.51
2:B:36:GLU:O	2:B:40:GLU:HG2	2.11	0.51
1:A:390:LYS:HE2	1:A:417:VAL:HG11	1.93	0.50
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.92	0.50
1:C:264:LEU:HD13	1:C:306:ASN:ND2	2.26	0.50
1:A:433:PRO:HG3	2:B:255:ASN:CB	2.41	0.50
2:B:221:HIS:CB	2:B:225:PRO:HG3	2.41	0.50
1:C:171:PHE:CE2	1:C:205:LEU:HA	2.47	0.50
2:D:419:THR:HG22	2:D:421:PRO:HD2	1.94	0.50
1:C:454:LYS:HE3	1:C:554:ALA:O	2.11	0.50
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.76	0.50
2:D:178:ILE:CG2	2:D:189:VAL:HG23	2.42	0.50
1:C:244:ILE:HG22	1:C:246:LEU:HD12	1.93	0.50
2:D:419:THR:CG2	2:D:421:PRO:HD2	2.40	0.50
1:A:50:ILE:HG21	1:A:145:GLN:HB3	1.94	0.50
1:A:439:THR:O	1:A:459:THR:HA	2.11	0.50
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.47	0.50
1:A:516:GLU:CD	1:A:516:GLU:H	2.19	0.50
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.94	0.50
1:C:524:GLN:O	1:C:528:LYS:HG2	2.12	0.50
1:A:275:LYS:HE2	1:A:332:GLN:OE1	2.12	0.50
1:A:281:LYS:HG3	1:A:284:ARG:NE	2.27	0.50
2:D:341:ILE:HD11	2:D:375:ILE:HG23	1.94	0.50
4:F:821:DC:H2'	4:F:822:DG:C8	2.47	0.50
1:C:199:ARG:HA	1:C:202:ILE:HB	1.94	0.50
1:C:407:GLN:NE2	2:D:418:ASN:HB3	2.27	0.49
1:A:54:ASN:O	1:A:143:ARG:NH2	2.45	0.49
1:A:443:ASP:OD1	1:A:444:GLY:N	2.41	0.49
1:A:448:ARG:O	1:A:451:LYS:NZ	2.39	0.49
2:B:266:TRP:CZ3	2:B:425:LEU:CB	2.95	0.49
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:GLU:O	2:D:339:TYR:HA	2.13	0.49
1:A:84:THR:HB	1:A:154:LYS:CE	2.31	0.49
2:B:285:GLY:H	2:B:287:LYS:NZ	2.11	0.49
1:C:199:ARG:CD	1:C:223:LYS:HE2	2.42	0.49
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.46	0.49
1:C:244:ILE:HD11	1:C:266:TRP:CD1	2.48	0.49
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.77	0.49
1:C:37:ILE:O	1:C:41:MET:HG3	2.13	0.49
1:C:42:GLU:CD	1:C:49:LYS:HE3	2.38	0.49
1:C:285:GLY:O	1:C:287:LYS:NZ	2.34	0.49
1:A:406:TRP:O	2:B:331:LYS:HB3	2.13	0.49
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.94	0.49
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.94	0.48
1:C:208:HIS:HD1	1:C:208:HIS:C	2.21	0.48
1:C:442:VAL:HG12	1:C:457:TYR:HB3	1.95	0.48
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.95	0.48
1:C:75:VAL:HB	1:C:77:PHE:CE2	2.48	0.48
1:C:181:TYR:CE2	2:D:138:GLU:HB2	2.47	0.48
1:A:390:LYS:HB3	1:A:417:VAL:CG1	2.43	0.48
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.49	0.48
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.95	0.48
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.78	0.48
1:C:28:GLU:HG2	1:C:135:ILE:HG23	1.95	0.48
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.39	0.48
1:A:427:TYR:CE2	1:A:525:LEU:HD13	2.48	0.48
1:C:107:THR:CG2	1:C:221:HIS:HE1	2.26	0.48
1:C:251:SER:O	1:C:252:TRP:CG	2.67	0.48
1:A:478:GLU:OE2	1:A:498:ASP:OD1	2.32	0.47
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.79	0.47
1:A:131:THR:OG1	1:A:143:ARG:HG2	2.14	0.47
2:D:23:GLN:OE1	2:D:59:PRO:HA	2.13	0.47
2:B:363:ASN:HB3	2:B:366:LYS:HB3	1.95	0.47
1:C:47:ILE:HD13	1:C:146:TYR:HA	1.97	0.47
1:C:486:LEU:CD1	1:C:521:ILE:HG23	2.44	0.47
1:A:30:LYS:HG2	1:A:62:ALA:O	2.15	0.47
1:A:285:GLY:N	3:T:715:DA:OP1	2.47	0.47
3:T:704:DA:C8	3:T:705:DT:H2'	2.49	0.47
1:A:301:LEU:HD23	1:A:301:LEU:O	2.15	0.47
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.50	0.47
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.44	0.47
1:A:275:LYS:HE2	1:A:332:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LYS:HE2	1:A:417:VAL:CG1	2.45	0.47
2:B:189:VAL:HG21	2:B:205:LEU:HD23	1.97	0.47
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.96	0.47
1:C:47:ILE:HG23	1:C:144:TYR:HB3	1.95	0.47
1:C:252:TRP:CD1	1:C:295:LEU:HD11	2.49	0.47
2:D:207:GLN:HA	2:D:210:LEU:HB3	1.96	0.47
1:A:228:LEU:CD2	1:A:233:GLU:HG2	2.45	0.47
2:B:125:ARG:HH11	2:B:147:ASN:HD22	1.62	0.47
2:D:317:VAL:HG13	2:D:347:LYS:HB3	1.97	0.47
1:C:97:PRO:HD3	1:C:232:TYR:CE2	2.50	0.47
1:C:442:VAL:HG21	1:C:482:ILE:HG12	1.97	0.47
2:D:214:LEU:C	2:D:229:TRP:HZ2	2.23	0.47
1:A:181:TYR:CD1	2:B:138:GLU:HG3	2.50	0.47
1:A:252:TRP:O	1:A:292:VAL:HG13	2.14	0.47
2:B:214:LEU:HD12	2:B:215:THR:H	1.79	0.47
2:B:216:THR:CG2	2:B:217:PRO:HD2	2.45	0.47
1:C:30:LYS:HG2	1:C:71:TRP:CZ3	2.50	0.47
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.97	0.46
2:D:82:LYS:HE2	2:D:413:GLU:CD	2.40	0.46
1:A:100:LEU:HD11	1:A:229:TRP:CZ3	2.51	0.46
1:A:329:ILE:O	1:A:392:PRO:HD3	2.15	0.46
1:C:275:LYS:HE2	1:C:332:GLN:CD	2.39	0.46
2:D:281:LYS:CB	2:D:284:ARG:NH1	2.78	0.46
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.96	0.46
1:A:524:GLN:O	1:A:528:LYS:HG2	2.15	0.46
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.16	0.46
2:D:200:THR:O	2:D:204:GLU:HG3	2.15	0.46
1:C:167:ILE:HD13	1:C:214:LEU:HD11	1.97	0.46
1:C:289:LEU:C	1:C:289:LEU:HD23	2.41	0.46
2:D:115:TYR:OH	2:D:157:PRO:HB3	2.15	0.46
2:D:168:LEU:HD22	2:D:180:ILE:HD13	1.96	0.46
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.98	0.46
1:A:235:HIS:HB3	1:A:238:LYS:HG2	1.97	0.46
1:C:66:LYS:H	1:C:72:ARG:HH21	1.62	0.46
1:C:128:THR:OG1	1:C:146:TYR:HB2	2.16	0.46
1:A:478:GLU:HG2	1:A:499:SER:CB	2.46	0.46
1:C:441:TYR:O	1:C:457:TYR:HA	2.16	0.46
1:C:458:VAL:HG12	1:C:464:GLN:HG2	1.98	0.46
3:E:704:DA:H2"	3:E:705:DT:C7	2.46	0.46
1:C:341:ILE:HD11	1:C:375:ILE:HG23	1.97	0.46
1:C:354:TYR:HD1	1:C:374:LYS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:GLN:O	2:D:211:ARG:HG2	2.16	0.46
1:A:253:THR:HA	1:A:291:GLU:O	2.16	0.46
1:C:440:PHE:N	1:C:494:ASN:O	2.41	0.46
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.98	0.46
1:A:26:LEU:HD21	1:A:61:PHE:HB3	1.96	0.45
1:C:422:LEU:HD12	1:C:422:LEU:N	2.31	0.45
1:C:439:THR:HA	1:C:494:ASN:O	2.16	0.45
1:A:94:ILE:HD11	4:P:819:DG:H21	1.81	0.45
1:A:254:VAL:HG23	1:A:291:GLU:HB3	1.98	0.45
1:A:376:THR:O	1:A:380:ILE:HG12	2.16	0.45
1:A:245:VAL:HG13	1:A:245:VAL:O	2.17	0.45
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.51	0.45
1:C:432:GLU:HA	1:C:432:GLU:OE1	2.16	0.45
2:D:100:LEU:HG	2:D:381:VAL:HG13	1.98	0.45
1:A:254:VAL:HG21	1:A:286:THR:CG2	2.47	0.45
1:C:257:ILE:HD11	1:C:295:LEU:HD21	1.98	0.45
1:A:46:LYS:HB3	1:A:148:VAL:HG21	1.97	0.45
2:B:28:GLU:OE2	2:B:32:LYS:HE3	2.17	0.45
2:B:253:THR:O	2:B:257:ILE:HG13	2.16	0.45
1:C:97:PRO:CD	1:C:232:TYR:CE2	2.99	0.45
1:C:231:GLY:CA	4:F:822:DG:H5'	2.47	0.45
1:C:498:ASP:OD2	1:C:538:ALA:HB2	2.17	0.45
2:D:281:LYS:CG	2:D:284:ARG:HH12	2.30	0.45
2:D:376:THR:HG23	2:D:386:THR:HG22	1.99	0.45
3:T:709:DC:H2'	3:T:710:DG:C8	2.51	0.45
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.45
1:A:208:HIS:O	1:A:212:TRP:HD1	1.99	0.45
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.98	0.45
2:B:281:LYS:CG	2:B:284:ARG:NH1	2.66	0.45
1:C:151:GLN:NE2	6:C:601:2NU:BR1	3.01	0.45
1:C:324:ASP:O	1:C:343:GLN:HG2	2.16	0.45
1:C:447:ASN:OD1	1:C:450:THR:HG23	2.17	0.45
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.47	0.45
2:D:47:ILE:HG22	2:D:146:TYR:HA	1.99	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.52	0.44
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.98	0.44
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.99	0.44
1:A:235:HIS:HE1	1:C:312:GLU:HG3	1.74	0.44
1:A:303:LEU:HD12	1:A:303:LEU:O	2.18	0.44
1:A:511:ASP:HA	1:A:522:ILE:HG21	2.00	0.44
1:C:31:ILE:HD12	1:C:135:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:CD1	1:C:266:TRP:CD1	3.00	0.44
1:C:246:LEU:HD12	1:C:246:LEU:N	2.32	0.44
2:D:160:PHE:O	2:D:160:PHE:CD1	2.70	0.44
1:C:73:LYS:NZ	1:C:146:TYR:OH	2.50	0.44
1:A:247:PRO:O	1:A:252:TRP:HH2	2.01	0.44
2:B:244:ILE:HG23	2:B:425:LEU:O	2.18	0.44
2:B:419:THR:HA	2:B:420:PRO:HD3	1.87	0.44
1:C:253:THR:HG22	1:C:289:LEU:O	2.18	0.44
1:C:91:GLN:C	1:C:92:LEU:HD22	2.43	0.44
1:C:95:PRO:HA	2:D:136:ASN:O	2.18	0.44
1:C:107:THR:O	1:C:189:VAL:N	2.45	0.44
1:C:442:VAL:HB	1:C:481:ALA:HB1	2.00	0.44
2:B:320:ASP:O	2:B:343:GLN:NE2	2.51	0.44
2:D:50:ILE:HD13	2:D:145:GLN:HB3	2.00	0.44
2:D:329:ILE:HD11	2:D:375:ILE:HD12	1.99	0.44
2:B:281:LYS:HD3	2:B:284:ARG:HH22	1.82	0.44
1:A:195:ILE:HG12	1:A:199:ARG:NH1	2.32	0.44
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.48	0.44
2:B:257:ILE:O	2:B:261:VAL:HG23	2.17	0.44
1:C:108:VAL:HB	1:C:222:GLN:CD	2.43	0.44
1:C:208:HIS:HA	1:C:211:ARG:HE	1.83	0.44
1:C:369:THR:HG22	1:C:411:ILE:HD11	1.99	0.44
1:C:486:LEU:HD12	1:C:521:ILE:HG23	2.00	0.44
2:D:332:GLN:CD	2:D:427:TYR:HB3	2.43	0.44
2:B:254:VAL:HG23	2:B:291:GLU:O	2.17	0.43
1:C:42:GLU:OE1	1:C:49:LYS:HE3	2.17	0.43
1:C:469:LEU:HD12	1:C:477:THR:HG22	1.99	0.43
1:A:34:LEU:HD11	1:A:61:PHE:HA	1.99	0.43
1:C:206:ARG:NE	1:C:216:THR:OG1	2.46	0.43
1:C:221:HIS:HE1	1:C:223:LYS:HD3	1.83	0.43
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.53	0.43
1:C:108:VAL:HA	1:C:187:LEU:O	2.19	0.43
1:C:429:LEU:HD11	1:C:506:ILE:HG22	1.99	0.43
1:A:225:PRO:HG3	1:A:227:PHE:HE2	1.82	0.43
2:B:38:CYS:O	2:B:47:ILE:HD11	2.18	0.43
1:C:105:SER:OG	1:C:195:ILE:HA	2.19	0.43
1:C:347:LYS:HD3	1:C:347:LYS:HA	1.83	0.43
2:D:111:VAL:N	2:D:185:ASP:O	2.46	0.43
2:D:132:ILE:HB	2:D:142:ILE:HG13	1.99	0.43
2:D:164:MET:HE2	2:D:187:LEU:CD1	2.48	0.43
1:A:359:GLY:HA2	4:P:810:DT:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:LYS:O	2:D:147:ASN:N	2.40	0.43
1:A:317:VAL:HG12	1:A:318:TYR:N	2.34	0.43
1:A:376:THR:HG23	1:A:386:THR:HG23	2.00	0.43
2:B:264:LEU:O	2:B:274:ILE:HG21	2.19	0.43
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.19	0.43
2:B:366:LYS:HE3	2:B:366:LYS:HB2	1.77	0.43
1:C:406:TRP:CZ3	2:D:420:PRO:HB3	2.53	0.43
2:D:266:TRP:CG	2:D:425:LEU:HD13	2.54	0.43
1:A:49:LYS:HG2	1:A:144:TYR:CE1	2.54	0.43
2:B:354:TYR:CZ	2:B:374:LYS:HE2	2.54	0.43
1:C:301:LEU:O	1:C:305:GLU:HG3	2.19	0.43
1:C:404:GLU:CD	1:C:431:LYS:HE3	2.44	0.43
1:A:379:SER:CB	1:A:387:PRO:HD3	2.49	0.42
2:D:420:PRO:CG	2:D:421:PRO:HD3	2.49	0.42
1:A:288:ALA:HB3	1:A:291:GLU:HB2	2.01	0.42
2:B:396:GLU:OE1	2:B:396:GLU:N	2.52	0.42
4:P:815:DG:H2'	4:P:816:DG:C8	2.54	0.42
1:C:114:ALA:HB1	1:C:160:PHE:CE2	2.54	0.42
1:C:164:MET:O	1:C:167:ILE:N	2.52	0.42
1:C:200:THR:O	1:C:204:GLU:HG3	2.18	0.42
1:C:254:VAL:HG13	1:C:255:ASN:N	2.34	0.42
1:C:292:VAL:HG13	1:C:292:VAL:O	2.19	0.42
2:D:356:ARG:HD2	2:D:356:ARG:HA	1.60	0.42
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.82	0.42
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.54	0.42
2:D:75:VAL:HG11	2:D:77:PHE:CZ	2.54	0.42
2:D:94:ILE:HG12	2:D:181:TYR:CE1	2.55	0.42
1:A:23:GLN:OE1	1:A:60:VAL:N	2.42	0.42
1:A:433:PRO:HG3	2:B:255:ASN:CG	2.44	0.42
1:C:264:LEU:HD21	1:C:306:ASN:HB3	2.00	0.42
1:C:277:ARG:HD2	1:C:336:GLN:CG	2.49	0.42
1:A:107:THR:CG2	1:A:221:HIS:HE1	2.32	0.42
2:B:81:ASN:CG	2:B:154:LYS:HB2	2.45	0.42
2:B:194:GLU:O	2:B:198:HIS:N	2.46	0.42
2:B:379:SER:HA	2:B:383:TRP:CE3	2.54	0.42
1:C:323:LYS:HE3	1:C:344:GLU:CG	2.48	0.42
1:C:390:LYS:HE2	1:C:417:VAL:HG11	2.02	0.42
2:B:215:THR:HG22	2:B:216:THR:N	2.33	0.42
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.49	0.42
1:A:266:TRP:O	1:A:269:GLN:HG2	2.20	0.42
2:B:50:ILE:HD13	2:B:145:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:VAL:HA	2:B:351:THR:O	2.19	0.42
1:C:7:THR:OG1	1:C:121:ASP:HA	2.19	0.42
1:C:66:LYS:HE2	1:C:66:LYS:HB3	1.89	0.42
1:C:257:ILE:O	1:C:261:VAL:HG22	2.20	0.42
1:C:323:LYS:HE3	1:C:344:GLU:OE2	2.19	0.42
1:C:496:VAL:HG21	2:D:289:LEU:HD21	2.01	0.42
1:A:254:VAL:CG2	1:A:293:ILE:CD1	2.98	0.42
1:C:452:LEU:HD23	1:C:470:THR:HA	2.02	0.42
2:D:107:THR:CB	2:D:202:ILE:HD11	2.50	0.42
1:A:54:ASN:O	1:A:143:ARG:CZ	2.68	0.42
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.50	0.42
1:C:65:LYS:HD3	1:C:68:SER:HB3	2.01	0.42
1:C:253:THR:O	1:C:257:ILE:HG12	2.20	0.42
1:C:274:ILE:HG12	1:C:309:ILE:HD11	2.01	0.42
4:F:808:DC:H2'	4:F:809:DC:C6	2.55	0.42
1:A:87:PHE:HD1	2:B:53:GLU:HA	1.85	0.41
1:A:511:ASP:OD1	1:A:512:LYS:HG2	2.20	0.41
2:D:210:LEU:HD12	2:D:210:LEU:HA	1.76	0.41
1:A:46:LYS:HB3	1:A:148:VAL:CG2	2.50	0.41
4:P:814:DC:H2''	4:P:815:DG:H8	1.83	0.41
1:C:244:ILE:HG23	1:C:263:LYS:CD	2.50	0.41
1:C:407:GLN:CD	2:D:418:ASN:HB3	2.45	0.41
2:D:319:TYR:CG	2:D:383:TRP:CD1	3.08	0.41
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.55	0.41
3:E:710:DG:H2'	3:E:711:DC:C6	2.54	0.41
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.94	0.41
2:D:24:TRP:CZ3	2:D:26:LEU:HD23	2.56	0.41
2:B:168:LEU:CD2	2:B:209:LEU:HD21	2.50	0.41
1:C:244:ILE:HD11	1:C:266:TRP:NE1	2.36	0.41
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.21	0.41
2:B:168:LEU:HD23	2:B:209:LEU:HD21	2.03	0.41
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.55	0.41
1:C:412:PRO:O	1:C:413:GLU:C	2.64	0.41
2:D:126:LYS:HE3	2:D:127:TYR:CZ	2.55	0.41
2:D:103:LYS:HA	2:D:192:ASP:OD1	2.19	0.41
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.55	0.41
1:C:156:SER:HB2	1:C:157:PRO:HD3	2.01	0.41
2:D:84:THR:HG22	2:D:85:GLN:N	2.35	0.41
2:D:121:ASP:OD1	2:D:123:ASP:OD1	2.38	0.41
1:A:185:ASP:OD2	4:P:822:DG:C5'	2.67	0.41
1:A:235:HIS:CD2	1:A:236:PRO:CD	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HA	1:A:284:ARG:HE	1.86	0.41
2:B:149:LEU:HD11	2:B:159:ILE:CG2	2.50	0.41
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.96	0.41
2:B:242:GLN:NE2	2:B:427:TYR:HD1	2.19	0.41
2:D:7:THR:HG22	2:D:119:PRO:HG2	2.03	0.41
1:A:34:LEU:HD21	1:A:61:PHE:O	2.21	0.41
1:A:497:THR:O	1:A:535:TRP:HA	2.20	0.41
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.95	0.41
2:B:266:TRP:CE3	2:B:425:LEU:CB	3.04	0.41
1:C:407:GLN:OE1	2:D:418:ASN:HA	2.21	0.41
1:C:498:ASP:CG	1:C:538:ALA:HB2	2.46	0.41
2:D:66:LYS:HB2	2:D:66:LYS:HE2	1.83	0.41
2:B:103:LYS:HD2	2:B:191:SER:C	2.46	0.40
1:C:121:ASP:OD2	1:C:123:ASP:HB2	2.20	0.40
1:C:164:MET:O	1:C:165:THR:C	2.65	0.40
2:D:65:LYS:HB2	2:D:68:SER:HB3	2.02	0.40
1:C:16:MET:HE2	1:C:16:MET:HB3	1.92	0.40
1:C:181:TYR:CD2	2:D:138:GLU:HG3	2.56	0.40
1:C:264:LEU:HD22	1:C:306:ASN:HB3	2.02	0.40
1:C:523:GLU:HG2	1:C:527:LYS:HE3	2.04	0.40
1:A:113:ASP:HB3	1:A:116:PHE:HB2	2.03	0.40
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.21	0.40
1:C:498:ASP:CB	1:C:538:ALA:HB2	2.49	0.40
1:C:179:VAL:O	1:C:180:ILE:HD13	2.22	0.40
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.22	0.40
1:A:46:LYS:HD2	1:A:116:PHE:O	2.21	0.40
1:A:160:PHE:CD1	1:A:160:PHE:C	2.99	0.40
1:C:90:VAL:HG23	2:D:140:PRO:HB3	2.04	0.40
1:C:377:THR:O	1:C:381:VAL:HG23	2.22	0.40
1:C:542:ILE:O	1:C:543:GLY:C	2.64	0.40

All (2) 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:B:199:ARG:NH2	3:T:717:DC:OP1[1_565]	1.98	0.22
1:C:6:GLU:OE1	2:D:121:ASP:OD2[2_455]	2.06	0.14

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	553/556 (100%)	539 (98%)	14 (2%)	0	100	100
1	C	549/556 (99%)	534 (97%)	14 (3%)	1 (0%)	43	71
2	B	414/444 (93%)	399 (96%)	15 (4%)	0	100	100
2	D	400/444 (90%)	385 (96%)	14 (4%)	1 (0%)	36	65
All	All	1916/2000 (96%)	1857 (97%)	57 (3%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	543	GLY
2	D	420	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	493/497 (99%)	492 (100%)	1 (0%)	87	88
1	C	492/497 (99%)	492 (100%)	0	100	100
2	B	373/403 (93%)	371 (100%)	2 (0%)	81	83
2	D	367/403 (91%)	363 (99%)	4 (1%)	65	76
All	All	1725/1800 (96%)	1718 (100%)	7 (0%)	84	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	GLU
2	B	358	ARG
2	B	411	ILE
2	D	86	ASP
2	D	92	LEU
2	D	191	SER
2	D	307	ARG

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

Mol	Chain	Res	Type
1	A	348	ASN
1	A	464	GLN
1	A	509	GLN
2	B	161	GLN
2	B	269	GLN
2	B	348	ASN
1	C	480	GLN
2	D	269	GLN
2	D	373	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 21 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	2NU	C	601	-	15,15,15	0.55	0	18,21,21	1.00	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2NU	C	601	-	-	6/12/14/14	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	2NU	C1-N1-C7	2.43	120.69	117.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	601	2NU	C2-C3-N2-C4
6	C	601	2NU	C2-C3-N2-N3
6	C	601	2NU	C8-C7-N1-C1
6	C	601	2NU	C8-C7-N1-C2
6	C	601	2NU	C9-C7-N1-C2
6	C	601	2NU	C9-C7-N1-C1

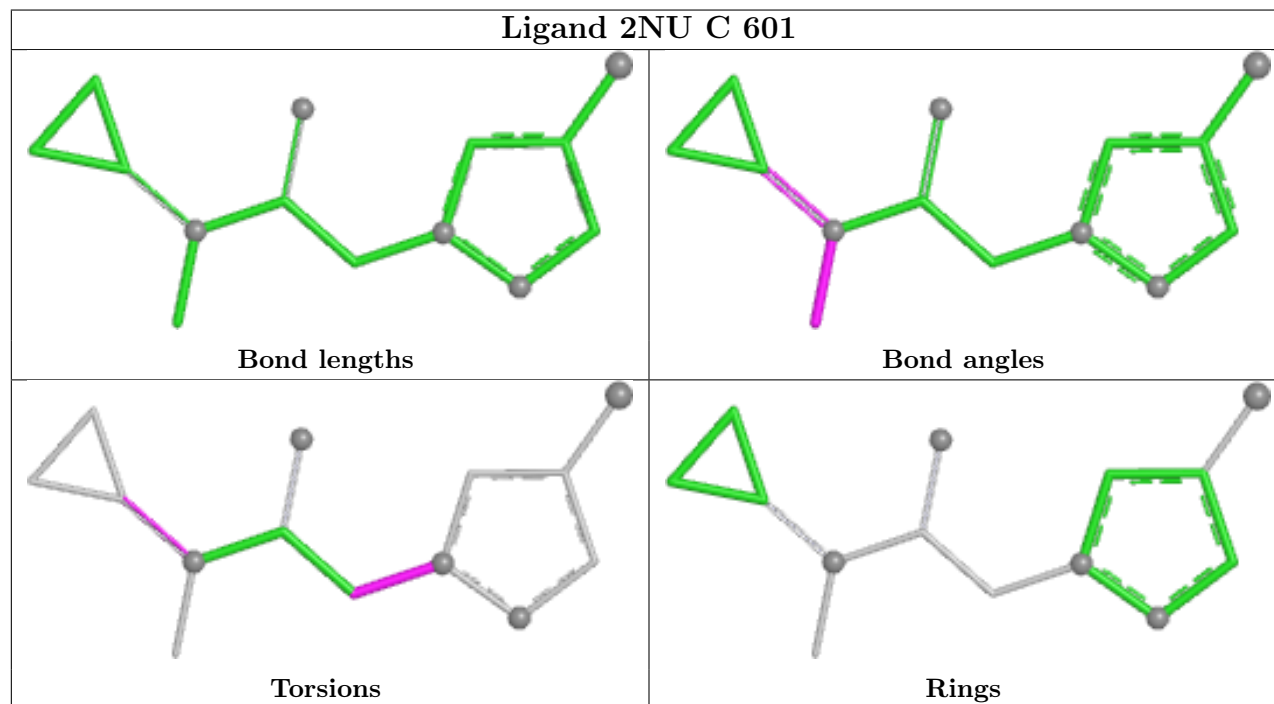
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	601	2NU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	555/556 (99%)	0.43	36 (6%)	25	17	22, 56, 124, 165	0
1	C	551/556 (99%)	0.51	34 (6%)	26	18	17, 63, 120, 174	0
2	B	418/444 (94%)	0.25	14 (3%)	49	33	18, 49, 101, 138	0
2	D	406/444 (91%)	0.38	17 (4%)	40	26	26, 53, 101, 180	0
3	E	22/28 (78%)	0.48	0	100	100	56, 85, 117, 122	0
3	T	23/28 (82%)	0.34	0	100	100	28, 73, 113, 152	0
4	F	20/21 (95%)	0.39	0	100	100	66, 85, 120, 131	0
4	P	21/21 (100%)	0.16	0	100	100	41, 57, 108, 130	0
All	All	2016/2098 (96%)	0.40	101 (5%)	34	23	17, 57, 117, 180	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	LEU	9.4
1	A	30	LYS	6.5
1	A	135	ILE	5.5
1	A	31	ILE	5.4
1	A	133	PRO	4.6
1	C	283	LEU	4.4
1	A	62	ALA	4.3
1	C	449	GLU	4.1
1	C	163	SER	3.9
1	C	202	ILE	3.6
1	C	522	ILE	3.6
1	A	198	HIS	3.5
1	A	124	PHE	3.4
2	D	232	TYR	3.4
1	A	61	PHE	3.4
2	B	357	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	28	GLU	3.3
1	A	138	GLU	3.3
1	C	404	GLU	3.3
1	A	26	LEU	3.3
1	A	545	ASN	3.3
1	C	209	LEU	3.2
1	A	27	THR	3.2
1	C	122	GLU	3.2
2	B	163	SER	3.2
1	C	34	LEU	3.1
2	D	346	PHE	3.1
2	D	354	TYR	3.1
1	C	170	PRO	3.1
1	A	140	PRO	3.0
2	B	168	LEU	3.0
2	D	428	GLN	3.0
1	A	77	PHE	3.0
1	C	198	HIS	3.0
1	C	24	TRP	2.9
1	A	134	SER	2.9
2	D	423	VAL	2.9
1	A	167	ILE	2.8
1	C	63	CYS	2.8
1	A	139	THR	2.8
1	C	62	ALA	2.8
1	A	74	LEU	2.7
2	B	384	GLY	2.7
1	A	24	TRP	2.7
1	C	66	LYS	2.7
2	B	172	LYS	2.7
1	A	80	LEU	2.7
1	A	178	ILE	2.7
1	A	60	VAL	2.7
1	A	180	ILE	2.6
1	A	73	LYS	2.6
1	A	111	VAL	2.6
1	A	33	ALA	2.5
2	B	360	ALA	2.5
2	D	425	LEU	2.5
1	C	261	VAL	2.5
2	B	115	TYR	2.5
1	A	235	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	299	ALA	2.5
1	A	274	ILE	2.5
1	A	475	GLN	2.4
2	D	426	TRP	2.4
2	D	93	GLY	2.4
2	D	107	THR	2.4
1	C	306	ASN	2.3
2	B	161	GLN	2.3
1	C	132	ILE	2.3
1	C	205	LEU	2.3
2	D	421	PRO	2.3
1	C	188	TYR	2.3
1	C	175	ASN	2.3
1	A	214	LEU	2.3
2	B	85	GLN	2.2
2	B	225	PRO	2.2
1	C	274	ILE	2.2
1	A	172	LYS	2.2
1	C	286	THR	2.2
2	D	405	TYR	2.2
1	C	529	GLU	2.2
2	B	226	PRO	2.2
1	C	551	LEU	2.2
1	C	396	GLU	2.1
1	C	402	TRP	2.1
2	D	90	VAL	2.1
1	A	149	LEU	2.1
1	C	264	LEU	2.1
2	D	193	LEU	2.1
1	A	394	GLN	2.1
1	C	409	THR	2.1
2	D	97	PRO	2.1
2	D	88	TRP	2.1
1	C	133	PRO	2.1
1	C	197	GLN	2.1
1	C	61	PHE	2.1
1	C	545	ASN	2.0
2	B	315	HIS	2.0
2	D	195	ILE	2.0
1	C	207	GLN	2.0
2	B	420	PRO	2.0
2	B	428	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	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](#)

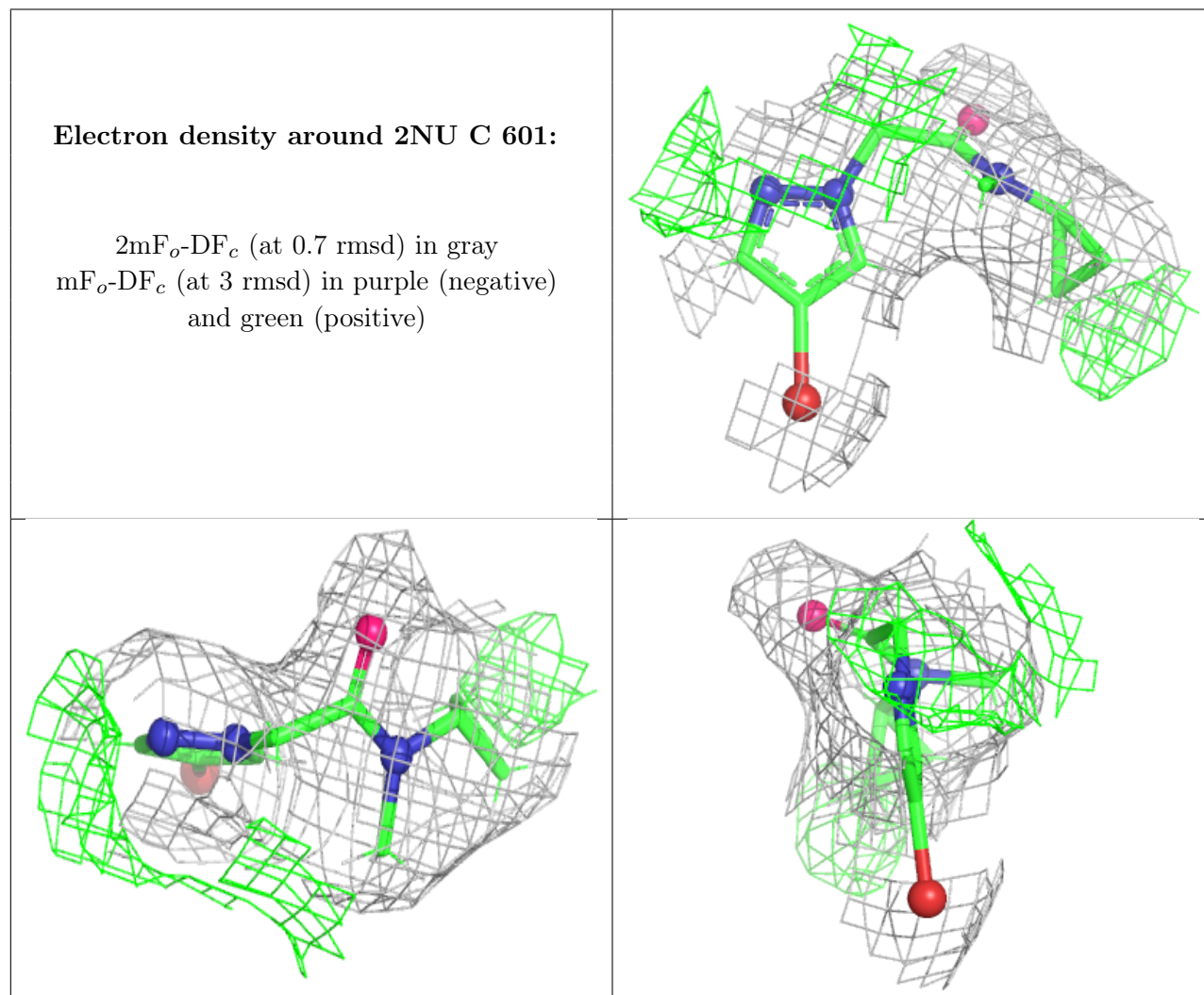
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
5	CD	E	801	1/1	0.69	0.12	144,144,144,144	0
5	CD	E	802	1/1	0.73	0.10	150,150,150,150	0
6	2NU	C	601	14/14	0.74	0.13	57,76,100,128	0
5	CD	T	802	1/1	0.78	0.09	154,154,154,154	0
5	CD	D	506	1/1	0.83	0.10	190,190,190,190	0
5	CD	B	502	1/1	0.85	0.14	203,203,203,203	0
5	CD	T	801	1/1	0.89	0.10	157,157,157,157	0
5	CD	B	501	1/1	0.89	0.14	102,102,102,102	0
5	CD	C	603	1/1	0.90	0.07	101,101,101,101	0
5	CD	C	604	1/1	0.93	0.09	178,178,178,178	0
5	CD	D	505	1/1	0.93	0.19	134,134,134,134	0
5	CD	D	503	1/1	0.96	0.05	118,118,118,118	0
5	CD	A	602	1/1	0.96	0.04	76,76,76,76	0
5	CD	A	603	1/1	0.96	0.04	99,99,99,99	0
5	CD	D	502	1/1	0.97	0.03	93,93,93,93	0
5	CD	B	503	1/1	0.97	0.15	143,143,143,143	0
5	CD	D	504	1/1	0.97	0.08	109,109,109,109	0
5	CD	P	901	1/1	0.97	0.03	103,103,103,103	0
5	CD	A	601	1/1	0.98	0.06	52,52,52,52	0
5	CD	C	602	1/1	0.99	0.04	40,40,40,40	0
5	CD	F	901	1/1	0.99	0.02	83,83,83,83	0
5	CD	D	501	1/1	0.99	0.02	51,51,51,51	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.