



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:31 AM UTC

PDB ID : 3V6D / pdb_00003v6d
Title : Crystal structure of HIV-1 reverse transcriptase (RT) cross-linked with AZT-terminated DNA
Authors : Das, K.; Martinez, S.E.; Arnold, E.
Deposited on : 2011-12-19
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

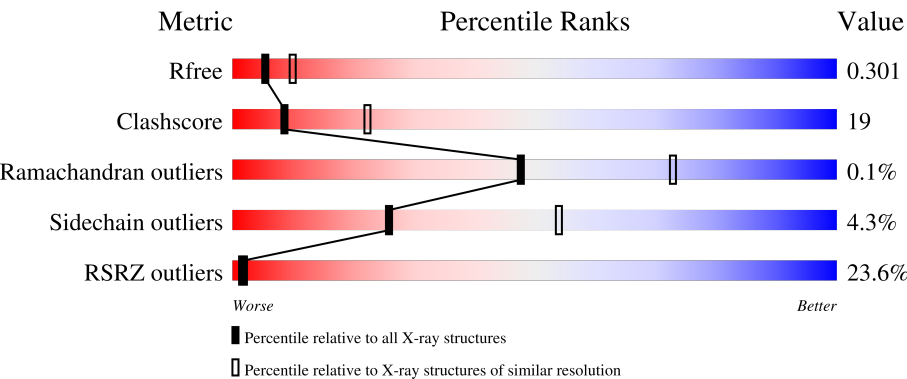
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	32% 60% 34% 5%
1	C	556	20% 57% 40% .
2	B	428	21% 64% 29% . .
2	D	428	19% 57% 36% . .
3	E	27	19% 33% 56% 11%

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Mol	Chain	Length	Quality of chain
3	T	27	22%37%52%11%
4	F	21	5%14%62%19%5%
4	P	21	19%29%48%19%5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17627 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 HIV-1 REVERSE TRANSCRIPTASE P66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4511	2920	751	832	8			
1	C	554	Total	C	N	O	S	0	0	0
			4506	2917	750	831	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	258	CYS	GLN	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
C	498	ASN	ASP	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 2 discrepancies between the modelled and reference sequences:

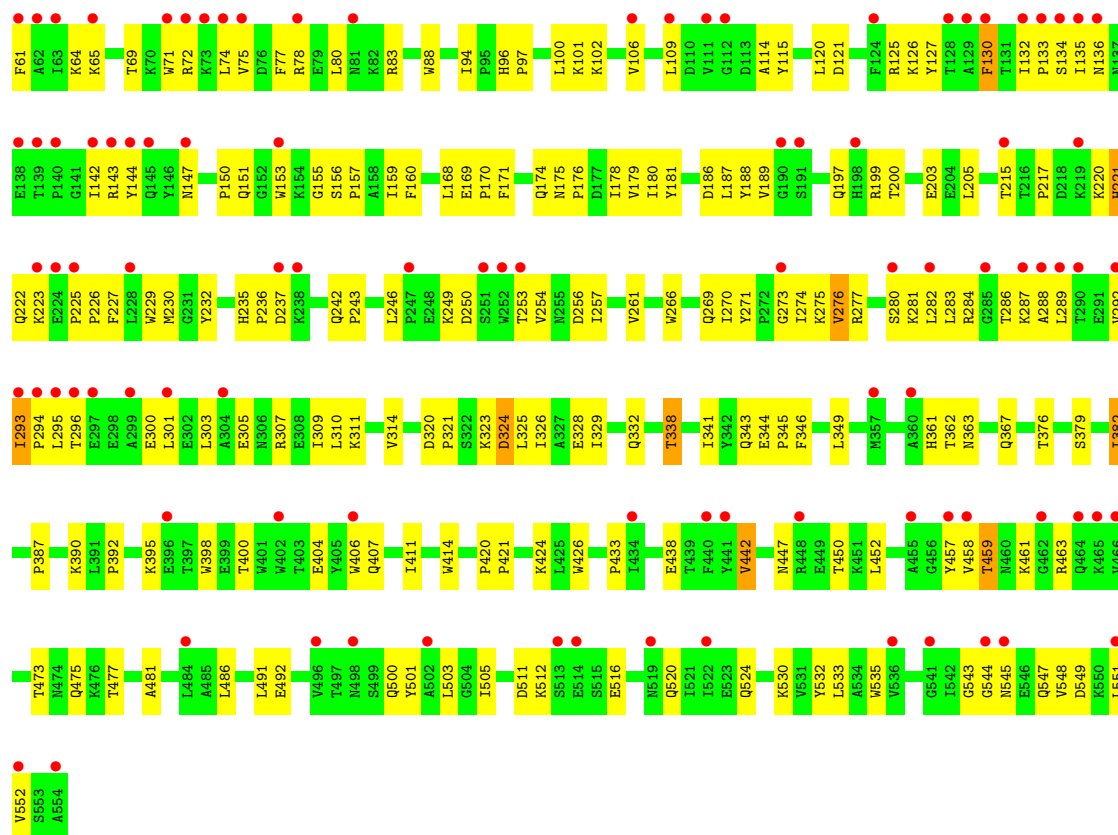
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

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

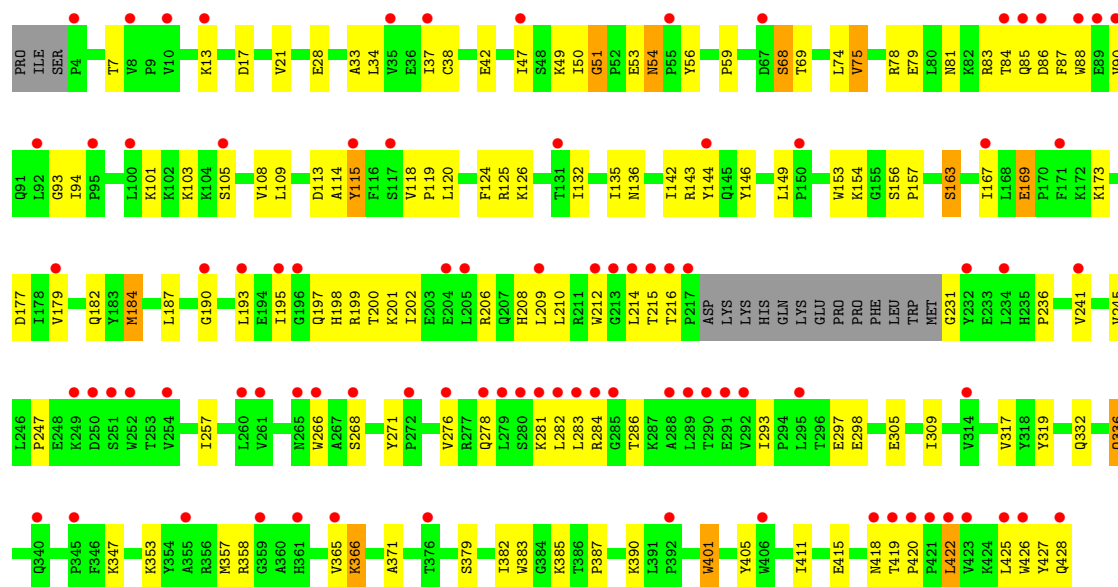
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	24	Total	C	N	O	P	0	0	0
			497	234	102	138	23			
3	E	24	Total	C	N	O	P	0	0	0
			497	234	102	138	23			

- 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*(MRG)P*CP*GP*CP*CP*(ATM))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	P	20	Total	C	N	O	P	S	0	0	0
			408	195	72	121	19	1			
4	F	20	Total	C	N	O	P	S	0	0	0
			408	195	72	121	19	1			



● Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit

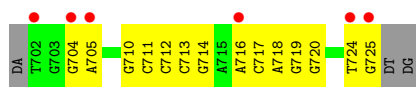


● Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit





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



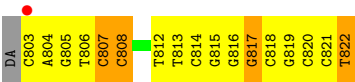
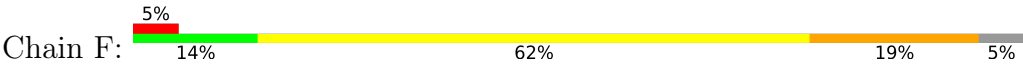
- Molecule 3: DNA (5'-D(*AP*TP*GP*GP*AP*AP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')



- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(M RG)P*CP*GP*CP*CP*(ATM))-3')



- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(M RG)P*CP*GP*CP*CP*(ATM))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.48Å 133.17Å 139.90Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	44.30 – 2.70 44.30 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.30-2.70) 97.8 (44.30-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.233 , 0.268 0.280 , 0.301	Depositor DCC
R_{free} test set	2607 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17627	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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

5.1 Standard geometry

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

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	0.60	0/4629	0.97	19/6290 (0.3%)
1	C	0.57	0/4624	0.93	14/6282 (0.2%)
2	B	0.62	0/3497	0.93	12/4751 (0.3%)
2	D	0.60	1/3497 (0.0%)	0.99	18/4751 (0.4%)
3	E	0.34	0/560	0.90	0/864
3	T	0.35	0/560	0.93	0/864
4	F	0.38	0/400	1.05	2/612 (0.3%)
4	P	0.34	0/400	1.04	2/612 (0.3%)
All	All	0.57	1/18167 (0.0%)	0.96	67/25026 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	423	VAL	CA-CB	5.23	1.59	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	422	LEU	N-CA-C	-10.02	100.19	111.71
2	D	54	ASN	CA-C-N	8.95	129.18	119.87
2	D	54	ASN	C-N-CA	8.95	129.18	119.87
1	A	4	PRO	N-CA-C	8.45	125.55	113.47
1	A	149	LEU	CA-C-N	8.37	128.13	119.76
1	A	149	LEU	C-N-CA	8.37	128.13	119.76
2	D	235	HIS	CA-C-N	8.06	127.79	119.56
2	D	235	HIS	C-N-CA	8.06	127.79	119.56
2	D	96	HIS	CA-C-N	7.91	129.73	119.84
2	D	96	HIS	C-N-CA	7.91	129.73	119.84
1	A	382	ILE	N-CA-C	7.89	118.48	110.82
1	C	54	ASN	CA-C-N	7.88	127.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ASN	C-N-CA	7.88	127.52	119.56
4	F	808	DC	C5'-C4'-C3'	-7.39	103.82	114.90
2	B	54	ASN	CA-C-N	7.04	127.19	119.87
2	B	54	ASN	C-N-CA	7.04	127.19	119.87
2	D	401	TRP	N-CA-C	6.87	121.95	113.50
2	B	401	TRP	N-CA-C	6.72	121.64	113.38
1	C	382	ILE	N-CA-C	6.71	117.33	110.82
4	P	808	DC	C5'-C4'-C3'	-6.68	104.89	114.90
1	A	3	SER	N-CA-C	6.62	123.61	108.93
2	D	195	ILE	N-CA-C	6.54	117.23	110.36
2	B	94	ILE	N-CA-C	6.37	114.83	107.89
1	A	132	ILE	N-CA-C	6.34	114.39	107.60
1	C	277	ARG	N-CA-C	6.32	118.73	111.02
1	C	51	GLY	CA-C-N	6.31	126.00	119.82
1	C	51	GLY	C-N-CA	6.31	126.00	119.82
2	D	51	GLY	CA-C-N	6.25	126.36	119.87
2	D	51	GLY	C-N-CA	6.25	126.36	119.87
2	B	51	GLY	CA-C-N	6.24	125.94	119.82
2	B	51	GLY	C-N-CA	6.24	125.94	119.82
1	A	2	ILE	N-CA-C	6.07	116.67	110.05
1	A	0	VAL	CA-C-N	6.01	126.51	120.14
1	A	0	VAL	C-N-CA	6.01	126.51	120.14
2	B	93	GLY	N-CA-C	5.83	120.06	112.25
1	C	276	VAL	N-CA-C	5.80	118.58	112.83
1	A	5	ILE	CB-CA-C	-5.77	103.78	111.80
1	A	237	ASP	N-CA-C	5.64	120.28	113.17
1	A	544	GLY	N-CA-C	-5.57	108.40	115.31
2	D	419	THR	CA-C-N	-5.56	114.65	120.38
2	D	419	THR	C-N-CA	-5.56	114.65	120.38
2	D	414	TRP	N-CA-C	5.54	117.68	108.99
2	B	68	SER	N-CA-C	5.52	117.10	111.14
1	C	237	ASP	N-CA-C	5.46	120.62	113.30
2	B	276	VAL	N-CA-C	5.45	118.22	112.83
1	C	8	VAL	CA-C-N	5.45	125.76	119.93
1	C	8	VAL	C-N-CA	5.45	125.76	119.93
1	C	5	ILE	CB-CA-C	-5.37	102.49	111.29
1	A	94	ILE	N-CA-C	5.36	114.38	108.05
4	F	807	DC	C4'-C3'-O3'	5.34	118.01	110.00
1	C	320	ASP	CA-C-N	5.32	125.64	119.47
1	C	320	ASP	C-N-CA	5.32	125.64	119.47
1	A	277	ARG	N-CA-C	5.31	116.75	110.97
2	D	424	LYS	N-CA-C	-5.26	106.45	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	MET	CB-CA-C	-5.24	110.55	116.63
2	D	343	GLN	N-CA-C	-5.19	106.08	112.72
1	A	132	ILE	CA-C-N	5.18	125.34	119.90
1	A	132	ILE	C-N-CA	5.18	125.34	119.90
2	D	284	ARG	N-CA-C	5.17	117.32	111.11
2	B	75	VAL	CA-C-N	-5.14	114.85	122.41
2	B	75	VAL	C-N-CA	-5.14	114.85	122.41
2	B	184	MET	CB-CA-C	-5.14	110.63	116.54
1	C	21	VAL	N-CA-C	5.05	115.64	108.42
2	D	85	GLN	N-CA-C	5.03	117.14	111.11
4	P	807	DC	C4'-C3'-O3'	5.02	117.53	110.00
1	A	246	LEU	CA-C-N	5.00	125.24	119.83
1	A	246	LEU	C-N-CA	5.00	125.24	119.83

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	4511	0	4570	175	0
1	C	4506	0	4568	187	0
2	B	3400	0	3433	118	0
2	D	3400	0	3433	140	0
3	E	497	0	268	14	0
3	T	497	0	268	15	0
4	F	408	0	231	27	0
4	P	408	0	231	20	0
All	All	17627	0	17002	655	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 19.

All (655) 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:223:LYS:O	1:C:225:PRO:HD3	1.53	1.09
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.41	1.01
2:D:13:LYS:HE3	2:D:16:MET:HE3	1.42	1.00
1:C:500:GLN:HG2	2:D:422:LEU:HD22	1.44	1.00
1:A:459:THR:HG22	1:A:461:LYS:H	1.23	0.99
1:A:2:ILE:H	1:A:2:ILE:HD12	1.26	0.99
1:A:223:LYS:O	1:A:225:PRO:HD3	1.64	0.98
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.01	0.96
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.31	0.94
1:A:37:ILE:HD12	1:A:40:GLU:HG3	1.52	0.91
1:A:65:LYS:HB3	1:A:68:SER:HB2	1.52	0.91
1:A:5:ILE:HG22	1:A:212:TRP:HD1	1.37	0.90
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.08	0.89
1:A:199:ARG:NH2	1:A:223:LYS:HB3	1.89	0.88
1:C:175:ASN:HB3	1:C:178:ILE:HD13	1.55	0.87
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.56	0.87
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.40	0.86
4:P:807:DC:H2''	4:P:808:DC:H5''	1.56	0.85
2:B:109:LEU:HD22	2:B:216:THR:HG21	1.59	0.84
1:C:450:THR:HG21	1:C:452:LEU:HD12	1.60	0.84
1:C:23:GLN:HE22	1:C:60:VAL:HG12	1.43	0.84
1:C:253:THR:HG22	1:C:292:VAL:HG12	1.60	0.83
1:C:199:ARG:NH2	1:C:223:LYS:HB2	1.93	0.83
4:F:817:MRG:N3	4:F:817:MRG:H222	1.94	0.81
2:B:13:LYS:HD2	2:B:85:GLN:HB3	1.63	0.80
1:C:303:LEU:O	1:C:307:ARG:HG3	1.81	0.79
1:A:303:LEU:O	1:A:307:ARG:HG3	1.83	0.79
2:B:266:TRP:NE1	2:B:425:LEU:HD22	1.98	0.79
2:D:87:PHE:HZ	2:D:159:ILE:HG13	1.48	0.79
1:A:199:ARG:HH21	1:A:223:LYS:HB3	1.47	0.78
1:C:438:GLU:OE2	1:C:459:THR:HG21	1.83	0.78
4:F:807:DC:H2''	4:F:808:DC:C5'	2.12	0.78
1:A:459:THR:CG2	1:A:461:LYS:H	1.97	0.78
4:P:807:DC:H2''	4:P:808:DC:C5'	2.14	0.78
2:D:266:TRP:CD1	2:D:425:LEU:HD22	2.18	0.78
4:F:807:DC:H2''	4:F:808:DC:H5''	1.65	0.77
1:A:459:THR:HG22	1:A:461:LYS:N	1.97	0.77
1:C:254:VAL:HG21	1:C:286:THR:HG21	1.65	0.77
1:C:459:THR:HG22	1:C:461:LYS:H	1.49	0.77
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.84	0.77
1:A:5:ILE:HG22	1:A:212:TRP:CD1	2.20	0.76
2:D:319:TYR:OH	2:D:385:LYS:HD2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LYS:HE2	1:C:344:GLU:OE2	1.85	0.76
2:D:266:TRP:NE1	2:D:425:LEU:HD22	2.00	0.76
2:B:281:LYS:HE3	2:B:284:ARG:NH2	2.01	0.76
1:C:459:THR:CG2	1:C:461:LYS:H	1.98	0.76
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.69	0.75
1:A:541:GLY:CA	1:A:546:GLU:HB2	2.16	0.75
2:B:182:GLN:HG3	2:B:187:LEU:HD12	1.68	0.75
1:A:78:ARG:HH21	3:T:705:DA:H5''	1.52	0.74
1:A:543:GLY:HA2	2:B:283:LEU:O	1.87	0.74
1:C:21:VAL:HG23	1:C:59:PRO:HD3	1.67	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.88	0.74
1:C:21:VAL:CG2	1:C:59:PRO:HD3	2.17	0.74
1:C:544:GLY:HA2	1:C:547:GLN:HE21	1.51	0.74
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.70	0.73
2:B:114:ALA:H	2:B:214:LEU:HD13	1.53	0.73
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.20	0.73
1:C:51:GLY:N	1:C:53:GLU:OE2	2.21	0.73
2:D:209:LEU:HD22	2:D:214:LEU:HD23	1.70	0.73
4:F:804:DA:H2'	4:F:805:DG:C8	2.24	0.73
3:E:721:DG:H2''	3:E:722:DA:OP2	1.87	0.72
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.71	0.72
1:A:511:ASP:OD2	1:A:512:LYS:NZ	2.21	0.72
2:B:33:ALA:O	2:B:37:ILE:HG12	1.89	0.72
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.52	0.72
1:A:252:TRP:O	1:A:292:VAL:HG23	1.90	0.72
2:D:358:ARG:HB2	2:D:370:GLU:OE2	1.90	0.72
1:A:66:LYS:NZ	1:A:67:ASP:OD2	2.24	0.71
1:A:125:ARG:HG2	1:A:146:TYR:O	1.91	0.71
1:A:543:GLY:N	2:B:283:LEU:O	2.23	0.71
2:B:68:SER:O	2:B:69:THR:HB	1.90	0.71
1:C:101:LYS:HE2	1:C:321:PRO:HG3	1.72	0.71
1:C:543:GLY:HA2	2:D:283:LEU:O	1.89	0.71
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.72	0.71
1:C:293:ILE:HG13	1:C:294:PRO:HD2	1.72	0.71
2:B:198:HIS:NE2	2:B:202:ILE:HD11	2.06	0.70
2:D:312:GLU:HB3	2:D:313:PRO:HD2	1.74	0.70
2:D:354:TYR:HE2	2:D:375:ILE:HG13	1.57	0.70
1:C:367:GLN:HE22	1:C:512:LYS:HD2	1.57	0.69
2:D:169:GLU:O	2:D:173:LYS:HG2	1.92	0.69
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.73	0.69
3:E:723:DC:H4'	3:E:723:DC:OP1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:723:DC:H5''	3:E:723:DC:H6	1.58	0.69
1:C:77:PHE:CD1	1:C:80:LEU:HD23	2.28	0.69
3:E:716:DA:H2''	3:E:717:DC:OP2	1.91	0.69
1:C:215:THR:HG22	1:C:217:PRO:HD3	1.74	0.68
2:D:342:TYR:HB3	2:D:348:ASN:HD22	1.57	0.68
1:A:544:GLY:O	1:A:548:VAL:HG23	1.94	0.68
1:A:253:THR:HA	1:A:292:VAL:HA	1.76	0.68
2:B:154:LYS:HG2	2:B:184:MET:SD	2.34	0.68
2:D:47:ILE:HD12	2:D:144:TYR:CD1	2.28	0.68
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.29	0.68
3:T:724:DT:H3	4:P:804:DA:H61	1.42	0.68
1:C:2:ILE:N	1:C:2:ILE:HD12	2.09	0.68
1:C:459:THR:HG22	1:C:461:LYS:N	2.08	0.68
2:D:157:PRO:HG3	2:D:184:MET:HA	1.75	0.68
2:D:266:TRP:HD1	2:D:425:LEU:HD13	1.59	0.68
2:D:360:ALA:HA	2:D:367:GLN:NE2	2.08	0.68
4:F:805:DG:H2''	4:F:806:DT:O5'	1.93	0.68
1:C:287:LYS:HG3	1:C:288:ALA:H	1.58	0.68
4:F:804:DA:H2''	4:F:805:DG:O5'	1.94	0.68
1:A:135:ILE:HG12	1:A:136:ASN:H	1.58	0.67
2:B:336:GLN:HG2	2:B:353:LYS:HD2	1.77	0.67
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.26	0.67
1:A:266:TRP:O	1:A:269:GLN:HG2	1.95	0.67
1:C:246:LEU:HD11	1:C:310:LEU:HD22	1.76	0.67
2:D:163:SER:O	2:D:167:ILE:HG13	1.94	0.67
1:A:41:MET:HB3	1:A:46:LYS:HB2	1.77	0.67
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.76	0.66
1:A:543:GLY:CA	2:B:283:LEU:O	2.43	0.66
2:B:332:GLN:HB2	2:B:336:GLN:HB3	1.76	0.66
1:C:109:LEU:HD23	1:C:220:LYS:HD2	1.77	0.66
2:D:86:ASP:OD1	2:D:87:PHE:N	2.29	0.66
2:D:214:LEU:HD12	2:D:215:THR:H	1.60	0.66
1:C:100:LEU:HD11	1:C:229:TRP:CZ3	2.31	0.66
2:D:16:MET:HG3	2:D:83:ARG:HG2	1.76	0.66
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.75	0.66
2:D:198:HIS:CD2	2:D:202:ILE:HD11	2.31	0.66
1:A:500:GLN:HG2	2:B:422:LEU:CD1	2.26	0.66
1:C:407:GLN:HE22	2:D:418:ASN:HA	1.60	0.66
1:C:32:LYS:O	1:C:36:GLU:HG3	1.97	0.65
4:F:803:DC:H2'	4:F:804:DA:C8	2.32	0.65
1:A:23:GLN:HG2	1:A:59:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:ALA:H	2:D:214:LEU:HD13	1.61	0.65
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.79	0.65
2:B:115:TYR:O	2:B:149:LEU:HB2	1.95	0.65
1:A:332:GLN:OE1	1:A:338:THR:HG23	1.96	0.65
4:P:817:MRG:N3	4:P:817:MRG:H222	2.12	0.65
1:C:289:LEU:HD21	4:F:817:MRG:H4'	1.77	0.64
1:C:543:GLY:O	1:C:547:GLN:NE2	2.30	0.64
4:F:806:DT:H2'	4:F:807:DC:C6	2.32	0.64
2:B:114:ALA:N	2:B:214:LEU:HD13	2.12	0.64
2:D:338:THR:HG22	2:D:353:LYS:HG3	1.80	0.64
1:A:253:THR:HG22	1:A:292:VAL:HB	1.79	0.64
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.13	0.64
1:C:21:VAL:HG22	1:C:57:ASN:O	1.98	0.64
1:C:500:GLN:HG2	2:D:422:LEU:CD2	2.23	0.64
4:F:807:DC:C2'	4:F:808:DC:H5''	2.28	0.63
1:C:503:LEU:CD1	1:C:533:LEU:HG	2.29	0.63
1:C:31:ILE:O	1:C:35:VAL:HG23	1.98	0.63
1:A:276:VAL:HG12	1:A:276:VAL:O	1.96	0.63
1:C:275:LYS:HE2	1:C:332:GLN:NE2	2.13	0.63
1:C:186:ASP:HB2	4:F:822:ATM:N5'	2.13	0.63
1:A:167:ILE:O	1:A:170:PRO:HD2	1.99	0.63
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.62	0.63
2:D:115:TYR:O	2:D:149:LEU:HB2	1.99	0.63
4:P:807:DC:H2'	4:P:808:DC:C6	2.33	0.63
1:A:78:ARG:NH2	3:T:705:DA:H5''	2.14	0.62
1:A:60:VAL:HG11	1:A:130:PHE:HD1	1.64	0.62
1:A:125:ARG:HE	1:A:147:ASN:HA	1.61	0.62
2:B:193:LEU:HB3	2:B:197:GLN:HB2	1.81	0.62
2:D:78:ARG:O	2:D:82:LYS:HG3	1.99	0.62
3:T:716:DA:H2''	3:T:717:DC:OP2	2.00	0.62
1:A:545:ASN:O	1:A:549:ASP:HB2	2.00	0.62
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.63	0.62
1:C:226:PRO:HB3	1:C:235:HIS:CE1	2.35	0.62
2:D:266:TRP:CD1	2:D:425:LEU:HD13	2.34	0.62
2:D:167:ILE:O	2:D:208:HIS:NE2	2.33	0.61
2:D:7:THR:HG22	2:D:119:PRO:HB2	1.82	0.61
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.24	0.61
1:C:395:LYS:NZ	1:C:414:TRP:O	2.34	0.61
1:A:61:PHE:CE1	3:T:704:DG:C8	2.89	0.61
2:B:169:GLU:O	2:B:173:LYS:HG2	2.00	0.60
1:A:500:GLN:HG2	2:B:422:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:718:DA:OP2	3:T:718:DA:H2'	2.02	0.60
1:C:307:ARG:O	1:C:311:LYS:HG3	2.00	0.60
1:A:254:VAL:HG21	1:A:286:THR:HG21	1.82	0.60
2:D:164:MET:HE1	2:D:209:LEU:HD21	1.83	0.60
1:A:135:ILE:CG2	1:A:138:GLU:HB2	2.31	0.60
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	2.90	0.60
4:F:807:DC:H2''	4:F:808:DC:O5'	2.01	0.60
1:C:61:PHE:HE1	1:C:74:LEU:HD12	1.67	0.59
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.84	0.59
1:C:109:LEU:CD2	1:C:220:LYS:HD2	2.32	0.59
2:D:40:GLU:HG2	2:D:44:GLU:OE1	2.02	0.59
2:B:86:ASP:OD1	2:B:87:PHE:N	2.35	0.59
1:C:37:ILE:O	1:C:40:GLU:HB2	2.02	0.59
3:T:725:DG:N2	4:P:803:DC:N3	2.39	0.59
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.37	0.59
1:C:516:GLU:O	1:C:520:GLN:HG3	2.03	0.59
2:D:109:LEU:HD22	2:D:216:THR:HG21	1.85	0.59
4:F:814:DC:H2''	4:F:815:DG:C8	2.38	0.59
1:A:5:ILE:CG2	1:A:212:TRP:HD1	2.10	0.58
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.37	0.58
1:A:452:LEU:HD23	1:A:470:THR:HA	1.84	0.58
2:B:317:VAL:HG12	2:B:347:LYS:CD	2.32	0.58
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.68	0.58
2:B:197:GLN:O	2:B:201:LYS:HG2	2.03	0.58
1:A:24:TRP:CD1	1:A:61:PHE:HE2	2.21	0.58
3:T:717:DC:H2''	3:T:718:DA:OP2	2.02	0.58
1:C:31:ILE:HG23	1:C:133:PRO:O	2.04	0.58
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.39	0.58
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.84	0.58
1:C:276:VAL:HG12	1:C:276:VAL:O	2.03	0.58
2:D:191:SER:OG	2:D:198:HIS:ND1	2.27	0.58
2:B:108:VAL:O	2:B:231:GLY:HA3	2.03	0.57
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.39	0.57
2:B:115:TYR:N	2:B:115:TYR:CD2	2.72	0.57
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.86	0.57
2:B:317:VAL:HG12	2:B:347:LYS:HD3	1.86	0.57
2:D:209:LEU:HD22	2:D:214:LEU:CD2	2.34	0.57
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.85	0.57
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.39	0.57
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.57
1:C:367:GLN:NE2	1:C:512:LYS:HD2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ARG:HH21	2:B:210:LEU:HD11	1.68	0.57
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.85	0.57
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.87	0.57
2:B:336:GLN:HG2	2:B:427:TYR:CE1	2.40	0.57
1:C:305:GLU:O	1:C:309:ILE:HG13	2.05	0.57
2:B:266:TRP:CD1	2:B:425:LEU:CD2	2.81	0.56
3:T:713:DC:H2''	3:T:714:DG:H5'	1.88	0.56
2:D:233:GLU:O	2:D:234:LEU:HD23	2.05	0.56
1:A:5:ILE:HD11	1:A:119:PRO:HD2	1.87	0.56
1:A:464:GLN:NE2	1:A:551:LEU:HD11	2.20	0.56
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.19	0.56
2:D:114:ALA:N	2:D:214:LEU:HD13	2.20	0.56
2:B:88:TRP:CZ2	2:B:154:LYS:HD2	2.40	0.56
2:D:118:VAL:HG12	2:D:119:PRO:O	2.05	0.56
3:E:704:DG:N3	3:E:704:DG:H5''	2.20	0.56
1:C:23:GLN:NE2	1:C:60:VAL:HG12	2.18	0.56
1:C:407:GLN:NE2	2:D:418:ASN:HA	2.20	0.56
1:A:139:THR:HG22	1:A:141:GLY:H	1.71	0.56
2:D:266:TRP:HE1	2:D:425:LEU:HD22	1.70	0.56
1:C:328:GLU:HG3	1:C:390:LYS:HB2	1.88	0.56
1:A:441:TYR:O	1:A:548:VAL:HG21	2.06	0.55
1:C:155:GLY:O	1:C:159:ILE:HG13	2.07	0.55
4:P:807:DC:C2'	4:P:808:DC:H5''	2.31	0.55
2:D:336:GLN:HG2	2:D:427:TYR:CE1	2.42	0.55
1:A:186:ASP:HB2	4:P:822:ATM:N5'	2.20	0.55
2:B:358:ARG:HG3	2:B:366:LYS:HD3	1.88	0.55
1:C:75:VAL:HB	1:C:77:PHE:CE2	2.42	0.55
1:C:473:THR:O	1:C:477:THR:HG23	2.06	0.55
2:D:160:PHE:O	2:D:160:PHE:CD2	2.60	0.55
2:B:115:TYR:N	2:B:115:TYR:HD2	2.05	0.55
1:A:523:GLU:O	1:A:527:LYS:HG3	2.06	0.55
2:D:168:LEU:HB3	2:D:172:LYS:HE3	1.88	0.55
4:F:815:DG:OP2	4:F:815:DG:H2'	2.07	0.55
1:A:37:ILE:HA	1:A:40:GLU:CG	2.37	0.54
4:P:815:DG:H2''	4:P:816:DG:O5'	2.05	0.54
1:A:206:ARG:NH2	1:A:216:THR:O	2.40	0.54
1:C:77:PHE:O	1:C:80:LEU:N	2.40	0.54
1:C:197:GLN:O	1:C:200:THR:HB	2.07	0.54
1:C:295:LEU:HD22	1:C:300:GLU:OE1	2.07	0.54
2:D:195:ILE:O	2:D:199:ARG:HG3	2.07	0.54
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:PRO:HD3	1:C:232:TYR:CE2	2.43	0.54
1:C:301:LEU:O	1:C:305:GLU:HG2	2.08	0.54
2:B:195:ILE:HG21	2:B:199:ARG:HH21	1.73	0.54
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.89	0.54
1:A:49:LYS:HE3	1:A:142:ILE:HG23	1.89	0.54
1:A:500:GLN:CD	2:B:422:LEU:HD11	2.32	0.54
1:A:132:ILE:HB	1:A:142:ILE:O	2.07	0.54
1:C:180:ILE:HA	1:C:188:TYR:O	2.07	0.54
2:D:425:LEU:HD23	2:D:426:TRP:CE2	2.42	0.54
1:A:516:GLU:O	1:A:520:GLN:HG3	2.08	0.54
1:C:130:PHE:CE2	1:C:144:TYR:HB2	2.43	0.53
1:C:287:LYS:HG3	1:C:288:ALA:N	2.23	0.53
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.89	0.53
2:D:56:TYR:HE2	2:D:126:LYS:HE2	1.73	0.53
2:D:175:ASN:OD1	2:D:201:LYS:NZ	2.34	0.53
4:F:817:MRG:H2'	4:F:818:DC:C6	2.43	0.53
1:C:406:TRP:CD1	1:C:407:GLN:HG2	2.44	0.53
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.07	0.53
1:C:503:LEU:HD11	1:C:533:LEU:HG	1.89	0.53
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.91	0.53
2:D:332:GLN:HB2	2:D:336:GLN:HB3	1.90	0.53
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.90	0.53
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.90	0.53
2:D:64:LYS:HE3	2:D:71:TRP:CZ2	2.44	0.53
2:B:281:LYS:HE3	2:B:284:ARG:HH21	1.74	0.53
2:D:87:PHE:CZ	2:D:159:ILE:HG13	2.37	0.53
3:T:713:DC:H2'	3:T:714:DG:C8	2.44	0.53
2:D:210:LEU:HA	2:D:214:LEU:O	2.09	0.53
2:D:395:LYS:HE2	2:D:399:GLU:OE2	2.08	0.53
1:A:123:ASP:OD2	1:A:123:ASP:N	2.42	0.52
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.91	0.52
1:A:135:ILE:HG23	1:A:138:GLU:HB2	1.90	0.52
2:B:105:SER:O	2:B:190:GLY:HA2	2.09	0.52
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.91	0.52
1:A:155:GLY:O	1:A:159:ILE:HG13	2.08	0.52
1:A:246:LEU:HD11	1:A:310:LEU:HD22	1.89	0.52
1:C:41:MET:HA	1:C:44:GLU:OE1	2.10	0.52
1:C:199:ARG:HE	1:C:222:GLN:HG2	1.72	0.52
2:D:16:MET:CG	2:D:83:ARG:HG2	2.39	0.52
2:D:111:VAL:HG23	2:D:115:TYR:HE1	1.74	0.52
1:A:31:ILE:HG21	1:A:135:ILE:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LYS:HE2	1:A:415:GLU:OE2	2.08	0.52
1:A:464:GLN:NE2	1:A:551:LEU:HD21	2.24	0.52
1:C:24:TRP:CZ3	3:E:703:DG:N2	2.76	0.52
2:D:360:ALA:C	2:D:362:THR:H	2.17	0.52
2:D:419:THR:O	2:D:420:PRO:C	2.50	0.52
1:C:257:ILE:HG21	1:C:283:LEU:HD21	1.90	0.52
1:C:398:TRP:CZ2	1:C:411:ILE:HG13	2.44	0.52
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.91	0.52
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.39	0.52
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.44	0.52
1:C:178:ILE:HD12	1:C:178:ILE:N	2.25	0.51
1:C:249:LYS:HG2	1:C:256:ASP:OD2	2.10	0.51
1:A:379:SER:CB	1:A:387:PRO:HD3	2.40	0.51
1:C:21:VAL:HG21	1:C:59:PRO:HD3	1.92	0.51
2:D:419:THR:O	2:D:419:THR:HG22	2.09	0.51
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.75	0.51
1:A:450:THR:HB	1:A:452:LEU:HD12	1.92	0.51
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.74	0.51
2:D:214:LEU:HD12	2:D:215:THR:N	2.25	0.51
1:C:362:THR:HG21	1:C:367:GLN:HE21	1.75	0.51
1:C:31:ILE:HD12	1:C:133:PRO:HB2	1.93	0.51
1:C:253:THR:CG2	1:C:292:VAL:HG12	2.36	0.51
2:D:198:HIS:O	2:D:202:ILE:HG13	2.10	0.51
1:C:10:VAL:O	1:C:11:LYS:HG3	2.11	0.51
4:F:806:DT:H2''	4:F:807:DC:OP1	2.09	0.51
1:A:169:GLU:N	1:A:170:PRO:HD2	2.25	0.51
1:C:126:LYS:HG3	1:C:127:TYR:CD2	2.46	0.51
1:C:186:ASP:CB	4:F:822:ATM:N5'	2.74	0.51
2:D:152:GLY:HA2	2:D:184:MET:HE3	1.93	0.51
4:F:804:DA:C2'	4:F:805:DG:C8	2.94	0.51
4:F:807:DC:H2'	4:F:808:DC:C6	2.46	0.51
2:D:210:LEU:HD12	2:D:214:LEU:O	2.11	0.50
4:F:817:MRG:N3	4:F:817:MRG:C22	2.72	0.50
2:D:73:LYS:CE	2:D:146:TYR:OH	2.60	0.50
2:B:87:PHE:C	2:B:87:PHE:CD2	2.88	0.50
2:D:109:LEU:HD22	2:D:216:THR:CG2	2.41	0.50
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.93	0.50
1:A:295:LEU:HB2	1:A:300:GLU:OE2	2.11	0.50
2:B:317:VAL:HG23	2:B:317:VAL:O	2.11	0.50
2:D:31:ILE:HD12	2:D:135:ILE:HG12	1.92	0.50
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:O	1:A:477:THR:HG23	2.12	0.50
2:D:167:ILE:HG23	2:D:212:TRP:CG	2.46	0.50
2:D:241:VAL:HG12	2:D:242:GLN:H	1.75	0.50
2:D:354:TYR:CE2	2:D:375:ILE:HG13	2.43	0.50
4:P:806:DT:H2'	4:P:807:DC:C6	2.47	0.50
2:B:101:LYS:O	2:B:236:PRO:HB2	2.12	0.50
4:P:803:DC:H2'	4:P:804:DA:C8	2.46	0.50
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.46	0.50
1:A:64:LYS:HE3	1:A:69:THR:O	2.11	0.50
1:C:94:ILE:HD11	3:E:708:DG:N2	2.26	0.50
1:C:179:VAL:O	1:C:189:VAL:HA	2.12	0.50
1:A:407:GLN:HE22	2:B:418:ASN:HA	1.76	0.49
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.94	0.49
2:B:305:GLU:O	2:B:309:ILE:HG13	2.11	0.49
1:A:63:ILE:O	1:A:72:ARG:HB3	2.12	0.49
1:A:184:MET:HG2	4:P:822:ATM:H1'	1.94	0.49
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.49
1:C:329:ILE:O	1:C:392:PRO:HD3	2.12	0.49
2:D:28:GLU:HA	2:D:135:ILE:HD11	1.93	0.49
1:A:37:ILE:HA	1:A:40:GLU:HG3	1.93	0.49
2:B:390:LYS:HE2	2:B:415:GLU:OE2	2.12	0.49
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.47	0.49
3:E:722:DA:H2''	3:E:723:DC:H5''	1.94	0.49
1:C:28:GLU:HB2	1:C:135:ILE:HG21	1.95	0.49
1:C:115:TYR:CD2	1:C:151:GLN:HG2	2.47	0.49
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.93	0.49
3:E:718:DA:H4'	3:E:719:DG:OP1	2.12	0.49
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.41	0.49
1:C:296:THR:O	1:C:300:GLU:HB2	2.12	0.49
4:F:819:DG:H2'	4:F:820:DC:C6	2.48	0.49
1:A:97:PRO:HD3	1:A:232:TYR:CE2	2.47	0.49
1:A:130:PHE:H	1:A:130:PHE:HD2	1.59	0.49
2:B:69:THR:O	2:B:69:THR:HG22	2.12	0.49
2:B:118:VAL:HG12	2:B:119:PRO:O	2.12	0.49
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.48	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.48	0.49
1:C:282:LEU:HB3	1:C:293:ILE:HD13	1.95	0.49
2:D:199:ARG:HA	2:D:202:ILE:HD12	1.94	0.49
1:A:17:ASP:OD2	1:A:56:TYR:HE1	1.96	0.49
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.48	0.49
1:A:10:VAL:HG12	1:A:11:LYS:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:GLN:CG	2:B:353:LYS:HD2	2.43	0.49
1:C:281:LYS:HG3	1:C:284:ARG:CZ	2.43	0.48
2:D:390:LYS:HE2	2:D:415:GLU:OE2	2.13	0.48
1:C:361:HIS:CD2	1:C:505:ILE:HG12	2.48	0.48
1:C:376:THR:HG21	2:D:401:TRP:CH2	2.48	0.48
1:A:2:ILE:CD1	1:A:2:ILE:N	2.73	0.48
1:C:223:LYS:O	1:C:223:LYS:HG2	2.13	0.48
1:C:276:VAL:HG12	1:C:280:SER:OG	2.12	0.48
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.96	0.48
2:B:281:LYS:O	2:B:284:ARG:HG3	2.14	0.48
1:A:2:ILE:H	1:A:2:ILE:CD1	1.99	0.48
1:C:37:ILE:HD13	1:C:40:GLU:HG3	1.96	0.48
1:C:50:ILE:HG12	1:C:54:ASN:HD22	1.79	0.48
1:A:10:VAL:HG12	1:A:11:LYS:N	2.29	0.48
1:A:24:TRP:O	1:A:26:LEU:HG	2.14	0.48
1:A:135:ILE:HG22	1:A:138:GLU:HB2	1.95	0.48
2:B:109:LEU:HD22	2:B:216:THR:CG2	2.37	0.48
1:C:324:ASP:O	1:C:343:GLN:HG2	2.13	0.48
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.48
2:B:206:ARG:NH2	2:B:210:LEU:HD11	2.29	0.48
1:C:130:PHE:H	1:C:130:PHE:HD2	1.60	0.48
1:C:171:PHE:CZ	1:C:205:LEU:HB2	2.49	0.48
2:D:85:GLN:HA	2:D:88:TRP:CE2	2.49	0.48
4:F:803:DC:H2'	4:F:804:DA:N7	2.28	0.48
2:B:56:TYR:HE2	2:B:126:LYS:CE	2.26	0.48
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.49	0.47
2:B:124:PHE:HE2	2:B:153:TRP:CZ2	2.32	0.47
4:P:811:DG:H2''	4:P:812:DT:O5'	2.14	0.47
1:C:37:ILE:HA	1:C:40:GLU:HG3	1.95	0.47
1:C:115:TYR:HD2	1:C:151:GLN:HG2	1.79	0.47
1:C:545:ASN:O	1:C:549:ASP:HB2	2.14	0.47
4:P:807:DC:H4'	4:P:808:DC:OP1	2.15	0.47
1:A:276:VAL:O	1:A:276:VAL:CG1	2.62	0.47
1:C:64:LYS:NZ	1:C:69:THR:HA	2.30	0.47
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.95	0.47
1:C:221:HIS:ND1	1:C:221:HIS:N	2.63	0.47
2:D:84:THR:HG22	2:D:84:THR:O	2.14	0.47
1:A:79:GLU:OE1	1:A:83:ARG:NH2	2.48	0.47
1:A:122:GLU:OE2	1:A:125:ARG:NH1	2.48	0.47
2:D:203:GLU:O	2:D:207:GLN:HG2	2.14	0.47
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HG22	1:A:276:VAL:HG13	1.97	0.47
1:A:500:GLN:CG	2:B:422:LEU:HD11	2.44	0.47
1:C:125:ARG:HH11	1:C:147:ASN:HB3	1.79	0.47
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.15	0.47
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.45	0.47
2:B:214:LEU:HD12	2:B:215:THR:H	1.80	0.47
1:C:102:LYS:HE2	1:C:236:PRO:O	2.14	0.47
1:C:406:TRP:CZ2	2:D:420:PRO:HG3	2.49	0.47
1:C:447:ASN:HB3	1:C:450:THR:HB	1.96	0.47
2:D:17:ASP:O	2:D:83:ARG:HD3	2.15	0.47
1:C:106:VAL:O	1:C:227:PHE:CZ	2.68	0.47
2:D:358:ARG:HB3	2:D:366:LYS:HE2	1.96	0.47
1:A:8:VAL:O	1:A:10:VAL:HG23	2.16	0.46
1:A:35:VAL:HA	1:A:38:CYS:HB2	1.97	0.46
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.50	0.46
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.97	0.46
1:A:106:VAL:O	1:A:227:PHE:CZ	2.68	0.46
1:A:135:ILE:HG12	1:A:136:ASN:N	2.27	0.46
1:A:228:LEU:HD22	1:A:242:GLN:NE2	2.31	0.46
1:C:65:LYS:HE2	1:C:72:ARG:HD3	1.98	0.46
1:C:242:GLN:HB3	1:C:243:PRO:HD2	1.96	0.46
1:C:398:TRP:CH2	1:C:411:ILE:HG13	2.50	0.46
1:A:88:TRP:CD1	2:B:143:ARG:NH1	2.84	0.46
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.30	0.46
1:C:64:LYS:HD3	1:C:71:TRP:CE2	2.50	0.46
1:C:120:LEU:HG	1:C:121:ASP:N	2.30	0.46
2:D:235:HIS:N	2:D:236:PRO:HD3	2.30	0.46
2:B:182:GLN:HG3	2:B:187:LEU:CD1	2.41	0.46
1:C:53:GLU:H	1:C:53:GLU:HG3	1.37	0.46
1:C:548:VAL:HA	1:C:551:LEU:HD12	1.98	0.46
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.51	0.46
2:D:13:LYS:HB3	2:D:14:PRO:HD2	1.98	0.46
4:F:815:DG:OP2	4:F:815:DG:H8	1.99	0.46
1:C:254:VAL:CG2	1:C:286:THR:HG21	2.42	0.46
2:D:41:MET:HB3	2:D:47:ILE:HG12	1.98	0.46
1:A:186:ASP:CB	4:P:822:ATM:N5'	2.78	0.46
1:C:88:TRP:CD1	2:D:143:ARG:NH1	2.83	0.46
1:C:169:GLU:N	1:C:170:PRO:HD2	2.31	0.46
1:C:345:PRO:O	1:C:346:PHE:HB2	2.15	0.46
1:A:100:LEU:HD11	1:A:229:TRP:CZ3	2.51	0.46
2:B:17:ASP:O	2:B:83:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.15	0.46
3:E:723:DC:H2''	3:E:724:DT:C6	2.51	0.46
2:B:197:GLN:O	2:B:200:THR:HB	2.16	0.45
2:B:379:SER:HB3	2:B:385:LYS:O	2.15	0.45
2:D:205:LEU:HD12	2:D:205:LEU:O	2.16	0.45
3:E:723:DC:H5''	3:E:723:DC:C6	2.46	0.45
1:A:424:LYS:HE3	1:A:426:TRP:CZ3	2.51	0.45
1:C:168:LEU:HD11	1:C:187:LEU:HD21	1.99	0.45
2:D:191:SER:HB2	2:D:193:LEU:HG	1.99	0.45
2:D:284:ARG:HG2	2:D:284:ARG:HH11	1.81	0.45
1:A:60:VAL:HG11	1:A:130:PHE:CD1	2.47	0.45
1:A:221:HIS:ND1	1:A:221:HIS:N	2.63	0.45
1:A:8:VAL:O	1:A:8:VAL:HG12	2.16	0.45
1:A:28:GLU:H	1:A:28:GLU:CD	2.24	0.45
1:A:131:THR:HA	1:A:143:ARG:HG2	1.98	0.45
1:C:420:PRO:HA	1:C:421:PRO:C	2.40	0.45
1:A:547:GLN:O	1:A:551:LEU:HB2	2.17	0.45
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.99	0.45
1:C:130:PHE:CD2	1:C:130:PHE:N	2.85	0.45
3:T:725:DG:N2	4:P:803:DC:C2	2.84	0.45
1:A:64:LYS:HD3	1:A:71:TRP:NE1	2.31	0.45
1:A:80:LEU:O	1:A:84:THR:OG1	2.29	0.45
1:A:553:SER:O	1:A:554:ALA:C	2.59	0.45
2:B:357:MET:HE1	2:B:371:ALA:HB2	1.98	0.45
1:C:64:LYS:HZ2	1:C:69:THR:HA	1.82	0.45
1:A:46:LYS:O	1:A:47:ILE:HG23	2.17	0.45
2:D:114:ALA:HB2	2:D:214:LEU:HD13	1.98	0.45
3:E:721:DG:C2'	3:E:722:DA:OP2	2.61	0.45
1:A:503:LEU:CD1	1:A:533:LEU:HD13	2.43	0.45
1:C:17:ASP:O	1:C:83:ARG:HD3	2.17	0.45
2:B:268:SER:HA	2:B:271:TYR:O	2.16	0.45
1:C:77:PHE:O	1:C:78:ARG:C	2.60	0.45
1:C:362:THR:CG2	1:C:367:GLN:HE21	2.29	0.45
3:E:706:DA:H2'	3:E:707:DG:C8	2.52	0.45
1:A:27:THR:OG1	1:A:29:GLU:HB3	2.17	0.44
1:A:60:VAL:CG1	1:A:130:PHE:HD1	2.27	0.44
2:B:247:PRO:CA	2:B:428:GLN:HE22	2.30	0.44
1:C:457:TYR:C	1:C:457:TYR:CD1	2.96	0.44
2:D:13:LYS:HD3	2:D:85:GLN:HB3	1.98	0.44
2:D:101:LYS:O	2:D:236:PRO:HB2	2.17	0.44
2:D:124:PHE:CE2	2:D:153:TRP:CZ2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:HG	1:C:121:ASP:H	1.82	0.44
2:D:78:ARG:HD3	2:D:411:ILE:O	2.17	0.44
2:D:323:LYS:O	2:D:385:LYS:NZ	2.50	0.44
1:A:77:PHE:O	1:A:80:LEU:N	2.49	0.44
2:D:109:LEU:HD23	2:D:109:LEU:HA	1.87	0.44
1:C:21:VAL:CG2	1:C:58:THR:HA	2.48	0.44
1:C:47:ILE:HG12	1:C:144:TYR:HB3	2.00	0.44
2:D:81:ASN:HB3	2:D:154:LYS:HD2	2.00	0.44
2:D:239:TRP:CH2	2:D:378:GLU:HA	2.53	0.44
2:D:317:VAL:HG23	2:D:317:VAL:O	2.17	0.44
4:P:818:DC:H2'	4:P:819:DG:H8	1.83	0.44
3:E:712:DC:H2''	3:E:713:DC:O5'	2.18	0.44
1:A:153:TRP:CD1	1:A:154:LYS:H	2.35	0.44
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.98	0.44
2:B:69:THR:O	2:B:69:THR:CG2	2.65	0.44
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.99	0.44
2:B:42:GLU:OE2	2:B:49:LYS:HG3	2.18	0.44
1:C:10:VAL:C	1:C:11:LYS:HG3	2.42	0.44
1:C:16:MET:CE	1:C:83:ARG:HG2	2.48	0.44
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.53	0.44
1:C:253:THR:HG22	1:C:292:VAL:CG1	2.39	0.44
3:T:710:DG:H2'	3:T:711:DC:C6	2.53	0.44
3:T:711:DC:H2''	3:T:712:DC:O5'	2.18	0.44
1:A:37:ILE:HA	1:A:40:GLU:HG2	1.98	0.44
1:C:424:LYS:HE2	1:C:426:TRP:CZ3	2.53	0.44
1:C:433:PRO:HD3	1:C:532:TYR:CZ	2.52	0.44
4:F:819:DG:H2'	4:F:820:DC:H6	1.83	0.44
1:A:197:GLN:O	1:A:200:THR:HB	2.18	0.44
2:B:195:ILE:O	2:B:199:ARG:HG3	2.18	0.44
1:A:420:PRO:HA	1:A:421:PRO:C	2.43	0.43
2:D:281:LYS:O	2:D:284:ARG:HG3	2.18	0.43
1:A:122:GLU:HB3	1:A:123:ASP:OD2	2.18	0.43
1:C:50:ILE:HD13	1:C:143:ARG:NH1	2.33	0.43
1:C:175:ASN:N	1:C:176:PRO:HD3	2.33	0.43
2:D:74:LEU:HD12	2:D:75:VAL:N	2.33	0.43
1:A:382:ILE:O	2:B:136:ASN:HB2	2.19	0.43
1:A:500:GLN:HG2	2:B:422:LEU:HD13	1.99	0.43
1:A:259:LYS:HG3	4:P:819:DG:OP1	2.17	0.43
1:C:254:VAL:HG21	1:C:286:THR:CG2	2.44	0.43
2:D:428:GLN:OE1	2:D:428:GLN:HA	2.18	0.43
1:A:130:PHE:CD2	1:A:130:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:CE1	1:A:175:ASN:ND2	2.86	0.43
1:A:277:ARG:HB3	1:A:336:GLN:OE1	2.19	0.43
2:B:157:PRO:HG3	2:B:184:MET:HA	1.99	0.43
2:D:198:HIS:NE2	2:D:202:ILE:HD11	2.33	0.43
1:A:451:LYS:O	1:A:471:ASN:N	2.51	0.43
1:C:27:THR:O	1:C:31:ILE:HG12	2.18	0.43
1:C:492:GLU:HG2	1:C:530:LYS:HB2	2.01	0.43
2:D:11:LYS:HA	2:D:11:LYS:HD3	1.83	0.43
1:C:1:PRO:HB2	1:C:2:ILE:H	1.59	0.43
1:C:132:ILE:HB	1:C:142:ILE:HG22	2.00	0.43
4:F:812:DT:H2''	4:F:813:DT:O5'	2.19	0.43
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.53	0.43
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.54	0.43
2:D:87:PHE:CD2	2:D:87:PHE:C	2.96	0.43
1:A:74:LEU:HD22	3:T:705:DA:C2	2.54	0.42
1:A:475:GLN:H	1:A:475:GLN:NE2	2.17	0.42
2:B:74:LEU:HD12	2:B:75:VAL:N	2.33	0.42
2:D:158:ALA:O	2:D:161:GLN:HB2	2.19	0.42
4:P:819:DG:H2'	4:P:820:DC:C6	2.53	0.42
2:B:210:LEU:HD23	2:B:214:LEU:O	2.18	0.42
1:C:2:ILE:HD12	1:C:2:ILE:H	1.84	0.42
1:C:325:LEU:HD23	1:C:325:LEU:HA	1.89	0.42
1:C:400:THR:O	1:C:404:GLU:HG2	2.20	0.42
2:D:209:LEU:HD13	2:D:214:LEU:HD23	2.02	0.42
1:A:464:GLN:HE21	1:A:551:LEU:HD21	1.82	0.42
1:C:491:LEU:HA	1:C:491:LEU:HD23	1.71	0.42
2:D:169:GLU:HB3	2:D:170:PRO:HD3	2.00	0.42
2:B:195:ILE:HG22	2:B:199:ARG:NE	2.33	0.42
1:C:58:THR:HG21	1:C:77:PHE:CE1	2.55	0.42
2:D:5:ILE:O	2:D:119:PRO:HG2	2.19	0.42
2:D:360:ALA:C	2:D:362:THR:N	2.75	0.42
2:B:34:LEU:HD23	2:B:34:LEU:HA	1.80	0.42
1:C:39:THR:HA	1:C:42:GLU:OE2	2.18	0.42
2:D:28:GLU:HG3	2:D:135:ILE:HD11	2.02	0.42
2:D:350:LYS:HE2	2:D:378:GLU:OE1	2.19	0.42
1:C:31:ILE:CG2	1:C:134:SER:HA	2.50	0.42
1:C:230:MET:O	4:F:821:DC:H5'	2.18	0.42
1:A:441:TYR:CD2	2:B:286:THR:HG23	2.55	0.42
1:A:401:TRP:HB2	1:A:425:LEU:HD11	2.02	0.42
1:C:486:LEU:HB3	1:C:524:GLN:HB3	2.02	0.42
2:D:120:LEU:HB3	2:D:147:ASN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:THR:O	2:D:203:GLU:HB3	2.20	0.42
1:A:454:LYS:HB2	1:A:552:VAL:O	2.19	0.42
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.01	0.42
2:B:317:VAL:HG12	2:B:347:LYS:HD2	2.02	0.42
2:B:419:THR:HG22	2:B:419:THR:O	2.18	0.42
1:C:150:PRO:HG2	1:C:153:TRP:HB2	2.02	0.42
1:A:41:MET:HB2	1:A:47:ILE:HD11	2.02	0.41
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.55	0.41
1:C:249:LYS:HD2	1:C:249:LYS:HA	1.81	0.41
2:D:207:GLN:HA	2:D:207:GLN:OE1	2.20	0.41
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.56	0.41
1:C:135:ILE:O	1:C:136:ASN:HB2	2.20	0.41
1:C:10:VAL:HG12	1:C:11:LYS:N	2.35	0.41
1:C:156:SER:HB2	1:C:157:PRO:HD3	2.01	0.41
1:C:326:ILE:O	1:C:341:ILE:HA	2.20	0.41
1:A:16:MET:CE	1:A:83:ARG:HG2	2.50	0.41
1:C:17:ASP:OD2	1:C:56:TYR:HE1	2.04	0.41
1:C:174:GLN:C	1:C:176:PRO:HD3	2.46	0.41
2:D:421:PRO:C	2:D:423:VAL:N	2.74	0.41
4:P:822:ATM:H6	4:P:822:ATM:O5'	2.21	0.41
2:B:425:LEU:HD23	2:B:426:TRP:CE2	2.56	0.41
1:C:261:VAL:CG1	1:C:276:VAL:HG11	2.47	0.41
1:C:458:VAL:HG23	1:C:548:VAL:HB	2.01	0.41
2:D:24:TRP:HZ2	2:D:61:PHE:CD2	2.39	0.41
3:T:719:DG:H2''	3:T:720:DG:C8	2.55	0.41
1:A:183:TYR:CE2	1:A:230:MET:HE1	2.55	0.41
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.76	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.41
2:B:210:LEU:HA	2:B:214:LEU:O	2.20	0.41
2:B:428:GLN:OE1	2:B:428:GLN:HA	2.21	0.41
1:C:36:GLU:O	1:C:40:GLU:HG2	2.21	0.41
1:C:266:TRP:O	1:C:269:GLN:HG2	2.20	0.41
2:D:10:VAL:HG13	2:D:87:PHE:CD1	2.55	0.41
1:A:23:GLN:HE21	1:A:23:GLN:HB3	1.64	0.41
1:C:31:ILE:HG21	1:C:134:SER:HA	2.02	0.41
1:C:171:PHE:CE2	1:C:205:LEU:HD13	2.55	0.41
1:C:271:TYR:CE1	1:C:314:VAL:HG22	2.55	0.41
1:A:21:VAL:N	1:A:57:ASN:O	2.48	0.41
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.50	0.41
2:D:168:LEU:CB	2:D:172:LYS:HE3	2.50	0.41
2:D:312:GLU:HB3	2:D:313:PRO:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.21	0.41
2:B:86:ASP:O	2:B:90:VAL:HB	2.21	0.41
2:B:382:ILE:HG22	2:B:383:TRP:CE2	2.56	0.41
1:C:60:VAL:HG11	1:C:130:PHE:HD1	1.85	0.41
1:C:535:TRP:CD2	2:D:422:LEU:HD21	2.56	0.41
2:D:73:LYS:HE3	2:D:146:TYR:OH	2.21	0.41
2:D:206:ARG:NH2	2:D:217:PRO:O	2.54	0.41
2:D:357:MET:HB3	2:D:370:GLU:OE1	2.21	0.41
4:F:815:DG:H2''	4:F:816:DG:OP2	2.21	0.41
1:A:326:ILE:O	1:A:341:ILE:HA	2.21	0.41
1:A:459:THR:CG2	1:A:460:ASN:N	2.84	0.41
2:B:81:ASN:CG	2:B:154:LYS:HG3	2.46	0.41
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.20	0.40
2:B:50:ILE:HG13	2:B:51:GLY:N	2.35	0.40
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.40
1:C:54:ASN:HA	1:C:55:PRO:HD2	1.86	0.40
1:C:120:LEU:CG	1:C:121:ASP:H	2.34	0.40
1:C:130:PHE:HD2	1:C:130:PHE:N	2.18	0.40
2:D:422:LEU:HA	2:D:422:LEU:HD12	1.77	0.40
2:B:53:GLU:HG2	2:B:54:ASN:N	2.35	0.40
2:B:297:GLU:OE1	2:B:297:GLU:HA	2.21	0.40
1:C:395:LYS:HD2	1:C:414:TRP:CH2	2.56	0.40
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.56	0.40
2:D:56:TYR:CE2	2:D:127:TYR:CE1	3.10	0.40
2:D:280:SER:O	2:D:281:LYS:C	2.63	0.40
1:A:134:SER:O	1:A:135:ILE:HB	2.19	0.40
2:B:84:THR:HG22	2:B:84:THR:O	2.22	0.40
2:D:142:ILE:HG22	2:D:144:TYR:CE2	2.56	0.40
1:A:135:ILE:HG22	1:A:138:GLU:CB	2.50	0.40
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.03	0.40
2:D:197:GLN:O	2:D:201:LYS:HG2	2.22	0.40
2:D:336:GLN:HE21	2:D:336:GLN:HB2	1.79	0.40
1:A:132:ILE:HD12	1:A:144:TYR:CD2	2.56	0.40
2:B:78:ARG:HD3	2:B:411:ILE:O	2.21	0.40
1:C:379:SER:CB	1:C:387:PRO:HD3	2.51	0.40
1:C:382:ILE:O	2:D:136:ASN:HB2	2.21	0.40
2:D:97:PRO:C	2:D:99:GLY:N	2.79	0.40
2:D:257:ILE:O	2:D:261:VAL:HG23	2.22	0.40
2:D:376:THR:HG21	2:D:410:TRP:CZ3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/556 (100%)	529 (96%)	23 (4%)	1 (0%)	43	68
1	C	552/556 (99%)	528 (96%)	24 (4%)	0	100	100
2	B	408/428 (95%)	399 (98%)	9 (2%)	0	100	100
2	D	408/428 (95%)	391 (96%)	17 (4%)	0	100	100
All	All	1921/1968 (98%)	1847 (96%)	73 (4%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/497 (100%)	465 (94%)	30 (6%)	17	40
1	C	495/497 (100%)	476 (96%)	19 (4%)	29	58
2	B	374/390 (96%)	360 (96%)	14 (4%)	30	59
2	D	374/390 (96%)	363 (97%)	11 (3%)	37	67
All	All	1738/1774 (98%)	1664 (96%)	74 (4%)	26	54

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	SER
1	A	5	ILE
1	A	8	VAL
1	A	23	GLN
1	A	28	GLU
1	A	35	VAL
1	A	36	GLU
1	A	39	THR
1	A	47	ILE
1	A	54	ASN
1	A	63	ILE
1	A	67	ASP
1	A	90	VAL
1	A	105	SER
1	A	123	ASP
1	A	130	PHE
1	A	188	TYR
1	A	221	HIS
1	A	248	GLU
1	A	292	VAL
1	A	293	ILE
1	A	324	ASP
1	A	338	THR
1	A	407	GLN
1	A	431	LYS
1	A	459	THR
1	A	523	GLU
1	A	529	GLU
1	A	548	VAL
2	B	113	ASP
2	B	115	TYR
2	B	163	SER
2	B	169	GLU
2	B	177	ASP
2	B	208	HIS
2	B	241	VAL
2	B	245	VAL
2	B	257	ILE
2	B	282	LEU
2	B	293	ILE
2	B	336	GLN
2	B	366	LYS

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Mol	Chain	Res	Type
2	B	422	LEU
1	C	2	ILE
1	C	3	SER
1	C	5	ILE
1	C	7	THR
1	C	47	ILE
1	C	50	ILE
1	C	53	GLU
1	C	130	PHE
1	C	203	GLU
1	C	221	HIS
1	C	250	ASP
1	C	270	ILE
1	C	274	ILE
1	C	293	ILE
1	C	324	ASP
1	C	338	THR
1	C	442	VAL
1	C	459	THR
1	C	552	VAL
2	D	58	THR
2	D	74	LEU
2	D	134	SER
2	D	135	ILE
2	D	241	VAL
2	D	248	GLU
2	D	336	GLN
2	D	379	SER
2	D	394	GLN
2	D	423	VAL
2	D	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	207	GLN
1	A	235	HIS
1	A	367	GLN
1	A	373	GLN
1	A	407	GLN
1	A	464	GLN

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Mol	Chain	Res	Type
1	A	487	GLN
1	A	520	GLN
2	B	208	HIS
2	B	269	GLN
2	B	278	GLN
2	B	336	GLN
1	C	54	ASN
1	C	222	GLN
1	C	373	GLN
1	C	407	GLN
1	C	464	GLN
1	C	498	ASN
1	C	524	GLN
1	C	545	ASN
1	C	547	GLN
2	D	145	GLN
2	D	315	HIS
2	D	348	ASN
2	D	361	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
4	MRG	F	817	1,3,4	25,28,29	2.57	8 (32%)	32,39,42	2.12	12 (37%)
4	ATM	F	822	3,4	20,23,24	1.27	2 (10%)	26,32,35	2.50	9 (34%)
4	ATM	P	822	3,4	20,23,24	1.28	2 (10%)	26,32,35	2.72	8 (30%)
4	MRG	P	817	1,3,4	25,28,29	2.64	8 (32%)	32,39,42	1.99	12 (37%)

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
4	MRG	F	817	1,3,4	-	3/12/26/27	0/3/3/3
4	ATM	F	822	3,4	-	1/10/24/25	0/2/2/2
4	ATM	P	822	3,4	-	1/10/24/25	0/2/2/2
4	MRG	P	817	1,3,4	-	3/12/26/27	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	817	MRG	C2-N2	6.62	1.48	1.34
4	P	817	MRG	C2-N2	6.51	1.48	1.34
4	F	817	MRG	C2-N3	6.09	1.43	1.32
4	P	817	MRG	C2-N3	5.98	1.43	1.32
4	P	817	MRG	C4-N3	4.65	1.44	1.34
4	F	817	MRG	C4-N3	4.46	1.44	1.34
4	P	817	MRG	C2-N1	4.43	1.43	1.36
4	F	817	MRG	C2-N1	4.08	1.43	1.36
4	P	817	MRG	C2'-C3'	-3.58	1.43	1.52
4	F	822	ATM	C6-C5	3.57	1.40	1.34
4	F	817	MRG	C2'-C3'	-3.54	1.43	1.52
4	P	817	MRG	O3'-C3'	-3.39	1.36	1.43
4	P	822	ATM	C4-C5	-3.17	1.39	1.44
4	P	822	ATM	C6-C5	3.09	1.39	1.34
4	F	817	MRG	O4'-C4'	-2.80	1.38	1.45
4	P	817	MRG	O4'-C4'	-2.73	1.38	1.45
4	F	817	MRG	O3'-C3'	-2.55	1.38	1.43
4	F	822	ATM	C4-C5	-2.34	1.41	1.44
4	P	817	MRG	O5'-C5'	-2.02	1.38	1.44
4	F	817	MRG	O5'-C5'	-2.01	1.38	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	822	ATM	C5-C4-N3	6.73	121.17	115.32
4	F	817	MRG	C2-N3-C4	6.27	119.85	112.00
4	F	822	ATM	C4-N3-C2	-6.25	119.14	127.34
4	P	822	ATM	C4-N3-C2	-6.03	119.43	127.34
4	P	817	MRG	C2-N3-C4	5.65	119.06	112.00
4	P	822	ATM	C2'-C1'-N1	-5.46	100.15	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	822	ATM	C5-C4-N3	5.15	119.80	115.32
4	F	817	MRG	C5-C4-N3	-4.73	120.87	128.39
4	P	822	ATM	O4-C4-C5	-4.65	119.60	124.92
4	F	822	ATM	N3-C2-N1	4.53	120.78	114.89
4	F	822	ATM	C5-C6-N1	-4.08	118.88	123.31
4	P	817	MRG	C5-C4-N3	-4.03	121.97	128.39
4	P	822	ATM	C5-C6-N1	-3.88	119.10	123.31
4	F	817	MRG	C2-N1-C6	-3.77	119.99	124.55
4	F	822	ATM	O4-C4-C5	-3.64	120.75	124.92
4	F	822	ATM	C6-C5-C4	3.46	120.87	118.02
4	P	822	ATM	N3-C2-N1	3.41	119.33	114.89
4	P	817	MRG	O4'-C1'-N9	3.32	113.76	107.86
4	P	822	ATM	O2-C2-N1	-3.16	118.68	122.80
4	F	817	MRG	O4'-C1'-N9	3.08	113.34	107.86
4	F	822	ATM	O2-C2-N1	-3.08	118.79	122.80
4	P	817	MRG	C2-N1-C6	-3.04	120.87	124.55
4	P	822	ATM	C5'-C4'-C3'	-2.71	106.22	114.27
4	P	817	MRG	C22-C21-N2	2.68	119.71	112.20
4	F	817	MRG	N9-C4-N3	2.63	131.21	125.95
4	P	817	MRG	N9-C8-N7	-2.56	108.65	113.40
4	F	817	MRG	C5-C6-N1	2.56	119.77	113.25
4	F	817	MRG	N9-C8-N7	-2.53	108.70	113.40
4	F	822	ATM	C5A-C5-C6	-2.44	119.55	122.85
4	F	817	MRG	O6-C6-C5	-2.39	120.23	126.53
4	F	817	MRG	C4-C5-N7	-2.36	106.93	110.67
4	P	817	MRG	O6-C6-C5	-2.36	120.31	126.53
4	P	817	MRG	N9-C4-N3	2.27	130.49	125.95
4	F	817	MRG	C22-C21-N2	2.23	118.46	112.20
4	P	817	MRG	C5-C6-N1	2.23	118.92	113.25
4	F	817	MRG	C8-N7-C5	2.19	108.17	104.26
4	F	822	ATM	O4'-C1'-N1	2.18	111.73	107.86
4	P	817	MRG	N1-C2-N3	-2.17	120.03	123.68
4	P	817	MRG	C4-C5-N7	-2.16	107.25	110.67
4	F	817	MRG	N1-C2-N3	-2.10	120.14	123.68
4	P	817	MRG	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	817	MRG	C22-C21-N2-C2
4	F	817	MRG	C22-C21-N2-C2

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Mol	Chain	Res	Type	Atoms
4	F	817	MRG	N2-C21-C22-C23
4	F	817	MRG	C21-C22-C23-S24
4	F	822	ATM	C3'-N3'-N4'-N5'
4	P	817	MRG	O4'-C4'-C5'-O5'
4	P	822	ATM	C4'-C3'-N3'-N4'
4	P	817	MRG	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	817	MRG	4	0
4	F	822	ATM	2	0
4	P	822	ATM	4	0
4	P	817	MRG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	1.70	178 (32%) 1 1	36, 83, 138, 149	0
1	C	554/556 (99%)	1.23	113 (20%) 3 2	34, 81, 136, 148	0
2	B	412/428 (96%)	1.37	88 (21%) 2 2	34, 66, 118, 131	0
2	D	412/428 (96%)	1.29	81 (19%) 3 2	40, 69, 125, 132	0
3	E	24/27 (88%)	1.28	5 (20%) 2 2	67, 104, 156, 164	0
3	T	24/27 (88%)	1.58	6 (25%) 2 1	69, 106, 158, 161	0
4	F	18/21 (85%)	1.04	1 (5%) 30 26	60, 92, 141, 142	0
4	P	18/21 (85%)	1.27	4 (22%) 2 2	68, 90, 142, 144	0
All	All	2017/2064 (97%)	1.40	476 (23%) 2 1	34, 75, 133, 164	0

All (476) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	THR	6.5
2	D	423	VAL	6.4
1	A	466	VAL	6.2
1	A	549	ASP	6.0
1	A	61	PHE	5.7
1	A	26	LEU	5.4
1	A	27	THR	5.4
1	A	133	PRO	5.4
1	A	74	LEU	5.4
2	D	354	TYR	5.3
2	B	88	TRP	5.1
2	D	232	TYR	5.0
2	D	420	PRO	5.0
1	A	152	GLY	5.0
2	B	214	LEU	4.9
1	A	459	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLY	4.9
1	C	71	TRP	4.8
1	C	132	ILE	4.8
2	B	215	THR	4.8
1	A	493	VAL	4.8
2	B	250	ASP	4.7
1	A	0	VAL	4.6
2	B	268	SER	4.6
1	C	466	VAL	4.5
2	B	359	GLY	4.5
2	B	252	TRP	4.5
2	B	422	LEU	4.4
2	D	360	ALA	4.4
2	B	425	LEU	4.4
2	D	217	PRO	4.3
1	C	133	PRO	4.3
1	A	70	LYS	4.3
2	B	291	GLU	4.3
2	D	357	MET	4.2
2	D	7	THR	4.2
1	C	464	GLN	4.2
2	B	213	GLY	4.2
1	A	548	VAL	4.2
2	B	86	ASP	4.1
1	A	441	TYR	4.0
1	A	439	THR	4.0
1	A	464	GLN	4.0
2	B	278	GLN	4.0
2	D	95	PRO	4.0
1	C	295	LEU	4.0
2	D	92	LEU	3.9
2	B	285	GLY	3.9
1	A	19	PRO	3.9
1	A	127	TYR	3.9
1	A	426	TRP	3.9
1	A	128	THR	3.8
1	C	61	PHE	3.8
1	C	552	VAL	3.8
1	A	448	ARG	3.8
1	A	551	LEU	3.8
1	C	135	ILE	3.8
1	A	140	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	204	GLU	3.8
2	D	187	LEU	3.8
1	A	37	ILE	3.8
2	D	15	GLY	3.8
1	A	38	CYS	3.7
2	B	212	TRP	3.7
1	C	129	ALA	3.7
1	C	144	TYR	3.7
1	C	223	LYS	3.7
2	B	292	VAL	3.7
1	A	494	ASN	3.7
1	C	247	PRO	3.7
1	C	143	ARG	3.7
1	A	451	LYS	3.6
1	A	33	ALA	3.6
2	D	212	TRP	3.6
2	B	8	VAL	3.6
1	A	118	VAL	3.5
2	B	117	SER	3.5
1	A	31	ILE	3.5
1	A	50	ILE	3.5
2	D	421	PRO	3.5
1	C	130	PHE	3.5
1	A	417	VAL	3.5
1	A	462	GLY	3.5
1	A	222	GLN	3.5
1	A	130	PHE	3.5
2	D	90	VAL	3.5
1	C	128	THR	3.4
1	A	440	PHE	3.4
1	A	552	VAL	3.4
1	A	495	ILE	3.4
1	A	542	ILE	3.4
1	A	145	GLN	3.4
2	D	426	TRP	3.4
1	C	251	SER	3.4
1	C	294	PRO	3.4
2	D	193	LEU	3.4
2	D	231	GLY	3.4
2	D	422	LEU	3.4
1	A	427	TYR	3.3
1	A	34	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	14	PRO	3.3
1	C	285	GLY	3.3
2	B	361	HIS	3.3
2	B	282	LEU	3.3
1	C	81	ASN	3.3
2	D	216	THR	3.3
1	C	112	GLY	3.3
1	C	554	ALA	3.3
1	A	527	LYS	3.3
1	A	468	PRO	3.3
1	C	134	SER	3.3
2	B	392	PRO	3.3
1	A	18	GLY	3.3
2	B	288	ALA	3.3
2	D	171	PHE	3.3
2	B	217	PRO	3.2
1	A	531	VAL	3.2
2	B	289	LEU	3.2
2	D	352	GLY	3.2
1	A	457	TYR	3.2
1	A	483	TYR	3.2
2	D	178	ILE	3.2
3	T	702	DT	3.2
1	C	145	GLN	3.2
1	C	191	SER	3.2
1	A	309	ILE	3.2
1	C	458	VAL	3.2
1	C	74	LEU	3.1
1	A	467	VAL	3.1
1	C	35	VAL	3.1
1	A	144	TYR	3.1
2	D	283	LEU	3.1
2	D	295	LEU	3.1
2	B	421	PRO	3.1
2	D	4	PRO	3.1
1	C	296	THR	3.1
1	C	299	ALA	3.1
1	A	35	VAL	3.1
1	A	149	LEU	3.1
2	B	209	LEU	3.1
1	A	23	GLN	3.1
1	C	502	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	251	SER	3.1
1	C	301	LEU	3.1
1	C	4	PRO	3.1
1	A	472	THR	3.1
1	A	132	ILE	3.1
2	B	249	LYS	3.1
1	A	259	LYS	3.0
1	C	455	ALA	3.0
2	D	88	TRP	3.0
2	D	118	VAL	3.0
1	C	448	ARG	3.0
1	A	543	GLY	3.0
2	D	362	THR	3.0
1	C	124	PHE	3.0
2	B	241	VAL	3.0
1	C	252	TRP	3.0
1	C	357	MET	3.0
2	B	345	PRO	2.9
2	D	242	GLN	2.9
2	B	284	ARG	2.9
1	C	288	ALA	2.9
2	D	355	ALA	2.9
2	D	241	VAL	2.9
1	A	71	TRP	2.9
2	B	232	TYR	2.9
1	C	5	ILE	2.9
2	B	195	ILE	2.9
1	A	39	THR	2.9
2	B	90	VAL	2.9
2	D	6	GLU	2.9
1	A	545	ASN	2.9
1	A	2	ILE	2.9
1	A	56	TYR	2.9
1	A	195	ILE	2.9
1	A	532	TYR	2.9
1	A	62	ALA	2.9
1	A	129	ALA	2.9
1	A	21	VAL	2.9
1	C	60	VAL	2.9
2	B	171	PHE	2.9
1	A	59	PRO	2.9
3	T	725	DG	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	47	ILE	2.9
1	A	318	TYR	2.9
1	A	335	GLY	2.9
1	A	442	VAL	2.9
1	A	47	ILE	2.8
1	C	142	ILE	2.8
2	B	260	LEU	2.8
2	B	254	VAL	2.8
2	D	198	HIS	2.8
1	A	430	GLU	2.8
4	P	803	DC	2.8
1	A	30	LYS	2.8
1	A	550	LYS	2.8
1	C	47	ILE	2.8
2	D	115	TYR	2.8
3	E	702	DT	2.8
2	D	94	ILE	2.8
2	D	109	LEU	2.8
1	A	465	LYS	2.7
2	B	167	ILE	2.7
1	A	535	TRP	2.7
2	B	279	LEU	2.7
1	A	436	GLY	2.7
2	D	361	HIS	2.7
2	B	84	THR	2.7
1	A	434	ILE	2.7
3	E	725	DG	2.7
1	A	443	ASP	2.7
1	C	287	LYS	2.7
2	B	92	LEU	2.7
2	D	214	LEU	2.7
2	B	190	GLY	2.7
1	C	7	THR	2.7
1	C	65	LYS	2.7
2	D	100	LEU	2.7
1	A	463	ARG	2.7
1	A	14	PRO	2.7
3	T	704	DG	2.6
2	D	425	LEU	2.6
4	F	803	DC	2.6
1	A	219	LYS	2.6
1	A	355	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	423	VAL	2.6
2	D	317	VAL	2.6
1	A	497	THR	2.6
1	A	63	ILE	2.6
1	A	12	LEU	2.6
1	C	72	ARG	2.6
1	A	220	LYS	2.6
1	A	447	ASN	2.6
1	C	545	ASN	2.6
1	A	139	THR	2.6
1	C	225	PRO	2.6
2	B	105	SER	2.6
1	A	332	GLN	2.6
1	A	480	GLN	2.6
2	D	284	ARG	2.6
1	A	414	TRP	2.6
2	D	197	GLN	2.6
1	A	274	ILE	2.6
2	D	274	ILE	2.6
2	B	420	PRO	2.6
1	A	227	PHE	2.6
1	A	200	THR	2.5
2	B	216	THR	2.5
2	D	266	TRP	2.5
1	A	5	ILE	2.5
1	A	135	ILE	2.5
2	B	37	ILE	2.5
2	B	150	PRO	2.5
1	A	343	GLN	2.5
2	B	418	ASN	2.5
2	D	5	ILE	2.5
2	B	234	LEU	2.5
2	B	283	LEU	2.5
1	C	140	PRO	2.5
1	A	90	VAL	2.5
1	A	496	VAL	2.5
1	C	75	VAL	2.5
2	B	179	VAL	2.5
1	C	62	ALA	2.5
2	B	419	THR	2.5
1	C	63	ILE	2.5
2	B	426	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	193	LEU	2.5
2	D	179	VAL	2.5
2	D	240	THR	2.5
1	C	484	LEU	2.5
2	D	105	SER	2.5
1	A	504	GLY	2.5
1	A	394	GLN	2.5
1	C	290	THR	2.4
2	B	290	THR	2.4
2	B	144	TYR	2.4
1	A	389	PHE	2.4
1	C	219	LYS	2.4
1	C	536	VAL	2.4
2	D	248	GLU	2.4
3	E	724	DT	2.4
1	C	273	GLY	2.4
1	C	544	GLY	2.4
1	C	440	PHE	2.4
1	A	69	THR	2.4
1	A	469	LEU	2.4
2	D	69	THR	2.4
1	A	81	ASN	2.4
1	A	198	HIS	2.4
1	C	224	GLU	2.4
1	A	55	PRO	2.4
2	B	340	GLN	2.4
2	B	261	VAL	2.4
1	A	299	ALA	2.4
1	A	554	ALA	2.4
2	D	299	ALA	2.4
1	A	283	LEU	2.4
1	A	295	LEU	2.4
1	A	325	LEU	2.4
1	A	473	THR	2.4
1	A	477	THR	2.4
2	D	419	THR	2.4
1	A	229	TRP	2.4
1	A	337	TRP	2.4
1	A	345	PRO	2.4
2	B	95	PRO	2.4
3	T	724	DT	2.4
2	B	355	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	434	ILE	2.3
1	C	3	SER	2.3
1	C	30	LYS	2.3
1	A	226	PRO	2.3
1	A	96	HIS	2.3
2	D	191	SER	2.3
1	A	4	PRO	2.3
1	A	247	PRO	2.3
1	C	106	VAL	2.3
2	B	100	LEU	2.3
3	E	703	DG	2.3
2	D	270	ILE	2.3
1	A	377	THR	2.3
2	B	115	TYR	2.3
1	C	498	ASN	2.3
1	C	19	PRO	2.3
2	B	55	PRO	2.3
2	B	67	ASP	2.3
1	C	153	TRP	2.3
1	A	241	VAL	2.3
2	D	87	PHE	2.3
2	D	168	LEU	2.3
1	A	470	THR	2.3
3	E	704	DG	2.3
1	C	136	ASN	2.3
1	A	121	ASP	2.3
2	B	280	SER	2.3
2	D	177	ASP	2.3
1	C	406	TRP	2.3
1	A	234	LEU	2.3
1	C	111	VAL	2.3
2	B	295	LEU	2.3
2	D	276	VAL	2.3
1	A	32	LYS	2.2
1	A	65	LYS	2.2
1	A	164	MET	2.2
1	A	386	THR	2.2
1	A	79	GLU	2.2
1	A	490	GLY	2.2
1	C	496	VAL	2.2
1	A	64	LYS	2.2
1	A	380	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	50	ILE	2.2
2	D	101	LYS	2.2
1	C	215	THR	2.2
1	C	396	GLU	2.2
1	A	1	PRO	2.2
1	A	243	PRO	2.2
1	C	25	PRO	2.2
1	A	547	GLN	2.2
2	D	280	SER	2.2
2	B	205	LEU	2.2
1	A	458	VAL	2.2
1	C	24	TRP	2.2
1	C	32	LYS	2.2
2	B	314	VAL	2.2
1	A	534	ALA	2.2
1	A	286	THR	2.2
1	C	139	THR	2.2
2	B	376	THR	2.2
2	D	286	THR	2.2
1	C	147	ASN	2.2
1	A	161	GLN	2.2
3	T	705	DA	2.2
3	T	716	DA	2.2
1	A	526	ILE	2.2
1	A	150	PRO	2.2
2	B	272	PRO	2.2
2	B	85	GLN	2.2
2	D	278	GLN	2.2
1	C	238	LYS	2.2
2	D	66	LYS	2.2
1	C	541	GLY	2.2
1	A	254	VAL	2.2
1	C	198	HIS	2.2
1	C	293	ILE	2.2
2	D	10	VAL	2.2
2	D	254	VAL	2.2
1	C	360	ALA	2.1
2	B	406	TRP	2.1
2	D	252	TRP	2.1
1	C	138	GLU	2.1
1	A	296	THR	2.1
1	C	14	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	13	LYS	2.1
2	B	265	ASN	2.1
1	A	342	TYR	2.1
1	A	205	LEU	2.1
1	A	525	LEU	2.1
2	B	35	VAL	2.1
2	B	365	VAL	2.1
2	D	165	THR	2.1
1	A	25	PRO	2.1
1	C	465	LYS	2.1
2	B	4	PRO	2.1
2	D	11	LYS	2.1
2	B	428	GLN	2.1
1	C	190	GLY	2.1
1	C	292	VAL	2.1
1	C	522	ILE	2.1
2	D	67	ASP	2.1
1	C	280	SER	2.1
1	A	288	ALA	2.1
1	A	360	ALA	2.1
2	B	89	GLU	2.1
2	B	266	TRP	2.1
2	D	239	TRP	2.1
1	A	376	THR	2.1
2	B	131	THR	2.1
2	B	281	LYS	2.1
1	A	486	LEU	2.1
1	C	282	LEU	2.1
1	A	498	ASN	2.1
1	C	441	TYR	2.1
1	C	462	GLY	2.1
2	D	375	ILE	2.1
4	P	816	DG	2.1
1	A	276	VAL	2.1
1	C	237	ASP	2.1
1	A	53	GLU	2.1
1	A	432	GLU	2.1
1	A	478	GLU	2.1
1	A	24	TRP	2.1
1	C	402	TRP	2.1
1	A	154	LYS	2.1
1	C	73	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	PRO	2.1
4	P	808	DC	2.1
1	A	301	LEU	2.1
1	A	261	VAL	2.1
2	B	10	VAL	2.1
1	C	78	ARG	2.0
1	C	514	GLU	2.0
2	D	353	LYS	2.0
1	C	253	THR	2.0
2	D	236	PRO	2.0
1	A	289	LEU	2.0
1	C	109	LEU	2.0
1	C	228	LEU	2.0
1	C	289	LEU	2.0
4	P	807	DC	2.0
1	A	460	ASN	2.0
1	C	2	ILE	2.0
2	D	195	ILE	2.0
1	A	60	VAL	2.0
1	A	271	TYR	2.0
2	D	108	VAL	2.0
1	C	297	GLU	2.0
1	C	22	LYS	2.0
1	C	304	ALA	2.0
2	D	281	LYS	2.0
1	C	513	SER	2.0
2	D	16	MET	2.0
1	A	392	PRO	2.0
1	C	34	LEU	2.0
1	C	551	LEU	2.0
1	A	175	ASN	2.0
1	A	456	GLY	2.0
1	A	541	GLY	2.0
1	C	519	ASN	2.0
2	B	196	GLY	2.0
2	D	190	GLY	2.0
2	B	276	VAL	2.0
1	A	146	TYR	2.0
1	A	319	TYR	2.0
1	C	457	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
4	MRG	P	817	26/27	0.79	0.13	88,102,117,121	0
4	ATM	P	822	22/23	0.82	0.13	71,82,95,95	0
4	MRG	F	817	26/27	0.82	0.12	84,99,117,127	0
4	ATM	F	822	22/23	0.88	0.13	71,78,87,95	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.