



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:34 pm BST

PDB ID : 3V6D
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

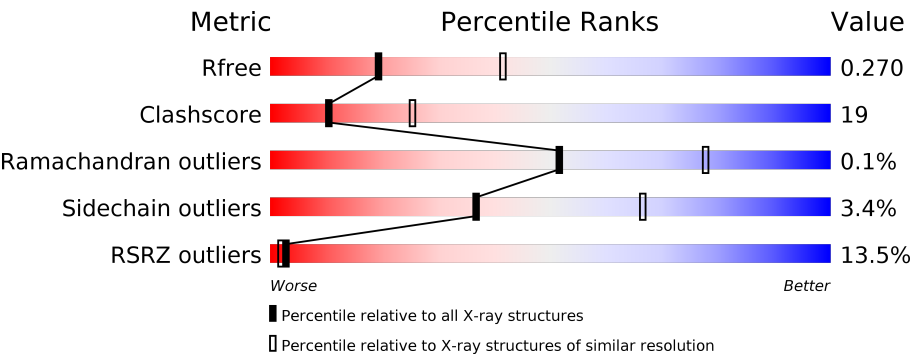
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div><div>17%</div><div><div></div><div>62%</div><div>35%</div><div>.</div></div></div>
1	C	556	<div><div>16%</div><div><div></div><div>58%</div><div>40%</div><div>.</div></div></div>
2	B	428	<div><div>7%</div><div><div></div><div>65%</div><div>30%</div><div>.</div><div>.</div></div></div>
2	D	428	<div><div>10%</div><div><div></div><div>60%</div><div>36%</div><div>.</div></div></div>
3	E	27	<div><div>19%</div><div><div>30%</div><div>37%</div><div>22%</div><div>11%</div></div></div>
3	T	27	<div><div>19%</div><div><div>26%</div><div>52%</div><div>11%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain				
4	F	21	<div><div></div><div></div><div></div><div></div><div></div></div> <div>10%5%62%29%5%</div>				
4	P	21	<div><div></div><div></div><div></div><div></div><div></div></div> <div>10%24%52%19%5%</div>				

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*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 497	C 234	N 102	O 138	P 23	0	0	0
3	E	24	Total 497	C 234	N 102	O 138	P 23	0	0	0

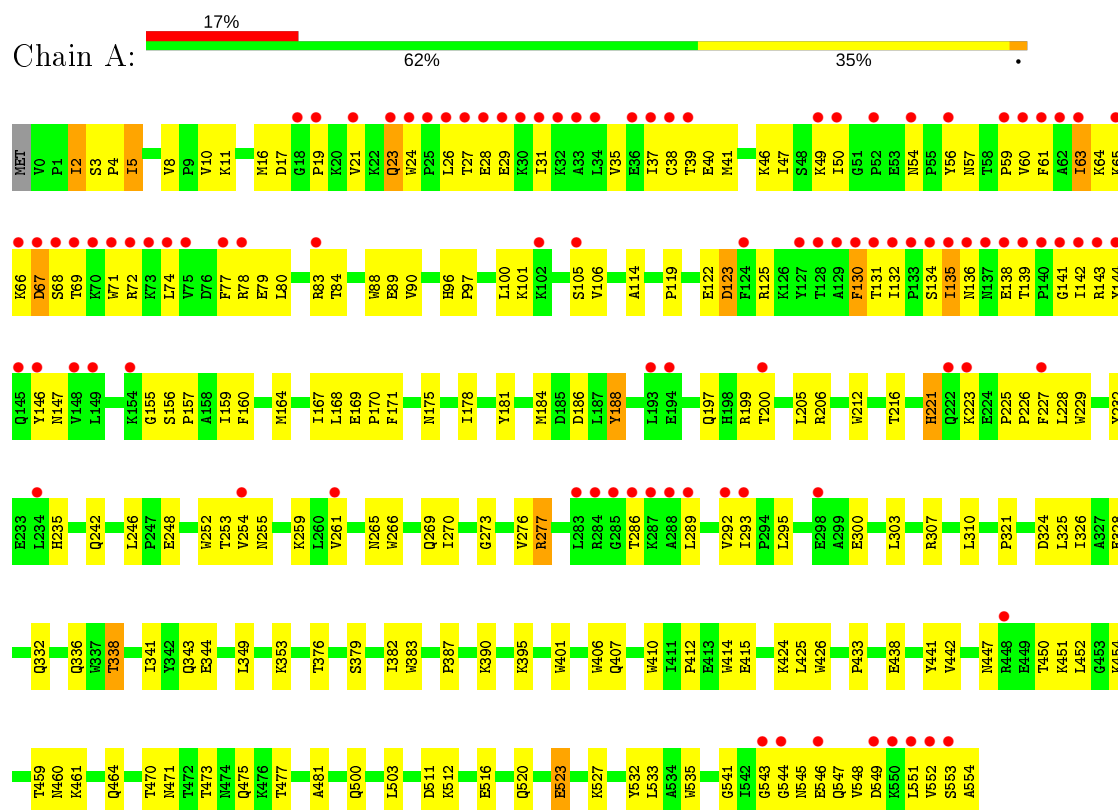
- Molecule 4 is a DNA chain called DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(ATM))-3').

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

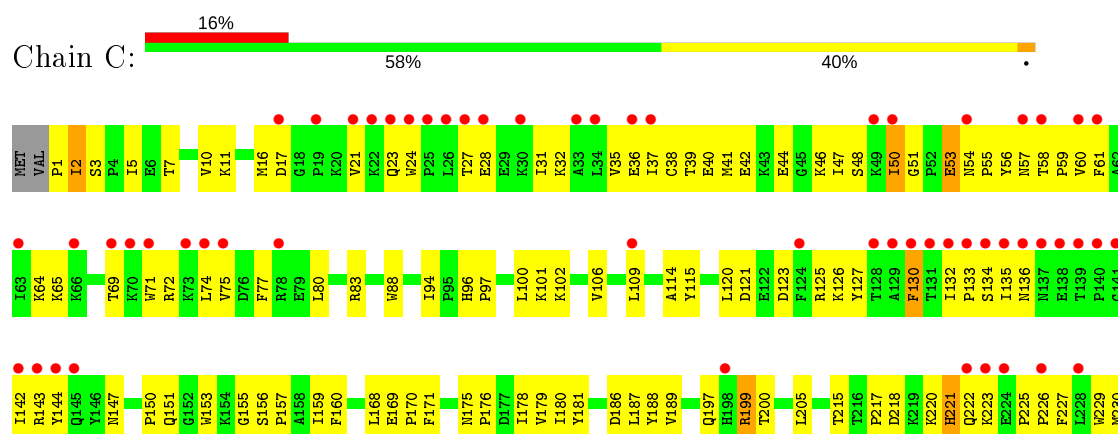
3 Residue-property plots [i](#)

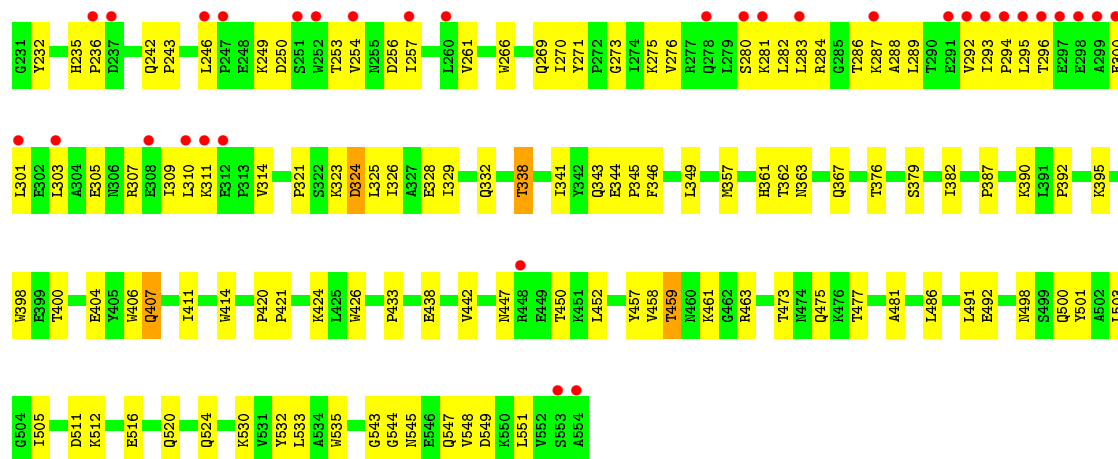
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 subunit

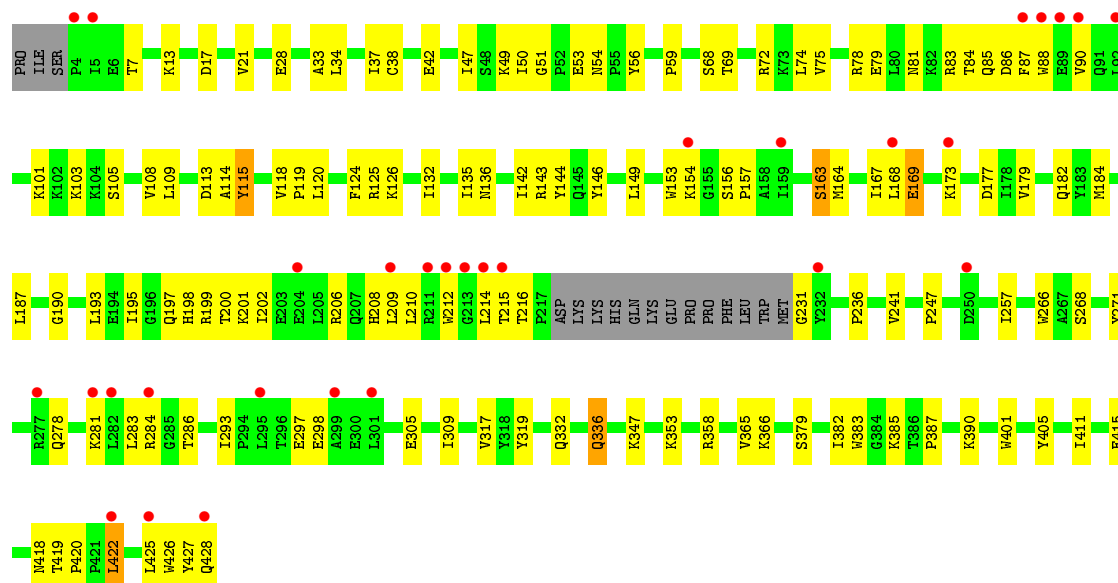


• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 subunit

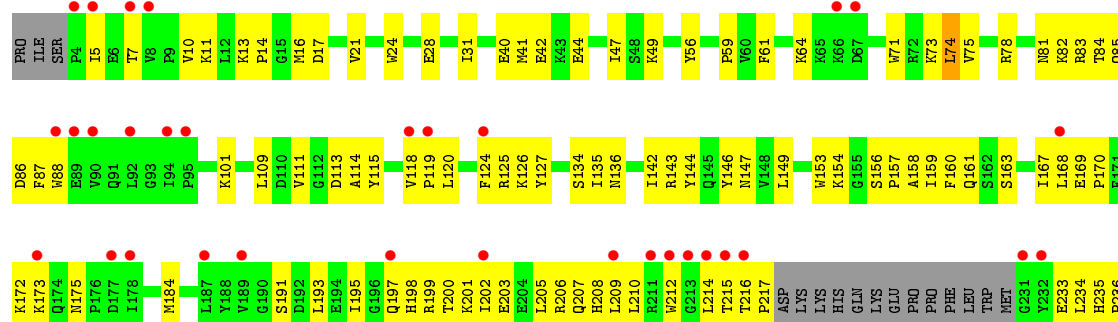


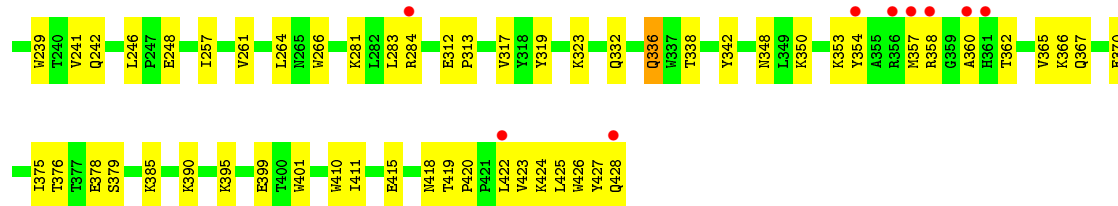


• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 subunit





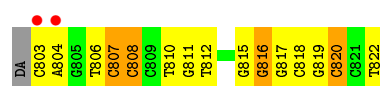
- Molecule 3: DNA (5'-D(*AP*TP*GP*GP*AP*AP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')



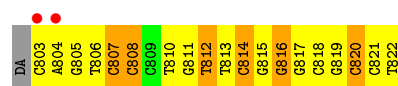
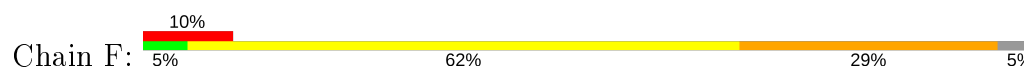
- Molecule 3: DNA (5'-D(*AP*TP*GP*GP*AP*AP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')



- 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 48.21 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.30-2.70) 97.8 (48.21-2.71)	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 0.234 , 0.270	Depositor DCC
R_{free} test set	2607 reflections (3.03%)	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 , 56.0	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	0.93	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/4629	0.61	1/6290 (0.0%)
1	C	0.45	0/4624	0.58	0/6282
2	B	0.48	0/3497	0.60	0/4751
2	D	0.46	0/3497	0.61	0/4751
3	E	0.79	0/560	1.44	10/864 (1.2%)
3	T	0.80	0/560	1.48	11/864 (1.3%)
4	F	0.82	0/400	1.58	9/612 (1.5%)
4	P	0.78	0/400	1.52	6/612 (1.0%)
All	All	0.51	0/18167	0.76	37/25026 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	810	DT	O4'-C1'-N1	9.89	114.92	108.00
4	F	807	DC	O4'-C1'-N1	8.96	114.27	108.00
4	P	816	DG	O4'-C1'-N9	8.78	114.14	108.00
3	E	721	DG	O4'-C1'-N9	-8.59	101.99	108.00
3	T	703	DG	O4'-C4'-C3'	-7.75	101.35	106.00
3	T	719	DG	C1'-O4'-C4'	-7.44	102.66	110.10
3	T	703	DG	O4'-C1'-N9	7.26	113.08	108.00
4	F	811	DG	O4'-C1'-N9	7.20	113.04	108.00
3	T	708	DG	O4'-C1'-N9	7.18	113.03	108.00
4	F	810	DT	N3-C4-O4	6.99	124.10	119.90
3	E	707	DG	O4'-C4'-C3'	-6.80	101.78	104.50
3	E	718	DA	O4'-C1'-N9	6.60	112.62	108.00
3	E	719	DG	C1'-O4'-C4'	-6.50	103.60	110.10
4	F	810	DT	C5-C4-O4	-6.46	120.38	124.90
3	T	708	DG	N9-C4-C5	6.41	107.96	105.40
4	F	812	DT	O4'-C1'-N1	-5.93	103.85	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	820	DC	O4'-C1'-N1	5.86	112.10	108.00
3	E	708	DG	N9-C4-C5	5.78	107.71	105.40
4	F	808	DC	C5'-C4'-C3'	-5.71	103.82	114.10
4	F	816	DG	O4'-C1'-N9	5.64	111.94	108.00
3	E	708	DG	C8-N9-C4	-5.62	104.15	106.40
4	P	807	DC	O4'-C1'-N1	5.55	111.89	108.00
3	E	703	DG	O4'-C1'-N9	5.55	111.88	108.00
3	E	711	DC	O4'-C1'-N1	5.49	111.84	108.00
3	T	708	DG	C8-N9-C4	-5.39	104.24	106.40
3	T	703	DG	C4'-C3'-C2'	-5.39	98.25	103.10
4	P	810	DT	C5-C4-O4	-5.33	121.17	124.90
4	F	820	DC	O4'-C1'-N1	5.23	111.66	108.00
3	E	707	DG	O4'-C1'-N9	5.18	111.63	108.00
3	T	718	DA	C3'-C2'-C1'	-5.18	96.28	102.50
4	F	814	DC	O4'-C1'-C2'	-5.18	101.76	105.90
1	A	4	PRO	N-CA-C	5.17	125.55	112.10
3	T	709	DC	C4'-C3'-C2'	-5.14	98.47	103.10
4	P	808	DC	C5'-C4'-C3'	-5.12	104.89	114.10
3	T	708	DG	C4'-C3'-C2'	-5.09	98.52	103.10
3	E	708	DG	N3-C2-N2	-5.06	116.36	119.90
3	T	720	DG	O4'-C1'-N9	-5.03	104.48	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4511	0	4570	174	0
1	C	4506	0	4568	182	0
2	B	3400	0	3433	117	0
2	D	3400	0	3433	135	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17627	0	17002	643	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 (643) 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
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:HD12	1:A:2:ILE:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OP1	3:E:723:DC:H4'	1.91	0.69
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:HD12	1:C:2:ILE:N	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:360:ALA:HA	2:D:367:GLN:NE2	2.08	0.68
2:D:266:TRP:HD1	2:D:425:LEU:HD13	1.59	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:214:LEU:HD12	2:D:215:THR:H	1.60	0.66
2:D:86:ASP:OD1	2:D:87:PHE:N	2.29	0.66
1:C:100:LEU:HD11	1:C:229:TRP:CZ3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:C:289:LEU:HD21	4:F:817:MRG:H4'	1.77	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:O	1:A:276:VAL:HG12	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:125:ARG:HE	1:A:147:ASN:HA	1.61	0.62
1:A:60:VAL:HG11	1:A:130:PHE:HD1	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:T:718:DA:H2'	3:T:718:DA:OP2	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:13:LYS:HB2	2:D:16:MET:HE3	1.82	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
2:D:13:LYS:HE3	2:D:16:MET:HE3	1.84	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:276:VAL:HG12	1:C:276:VAL:O	2.03	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:114:ALA:HB1	1:C:160:PHE:CZ	2.39	0.58
1:C:31:ILE:HG23	1:C:133:PRO:O	2.04	0.58
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.84	0.58
2:D:191:SER:OG	2:D:198:HIS:ND1	2.27	0.58
2:B:115:TYR:CD1	2:B:156:SER:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TYR:CD2	2:B:115:TYR:N	2.72	0.57
2:B:108:VAL:O	2:B:231:GLY:HA3	2.03	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
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.57
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.39	0.57
1:C:367:GLN:NE2	1:C:512:LYS:HD2	2.18	0.57
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:D:13:LYS:HE3	2:D:16:MET:CE	2.34	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:464:GLN:NE2	1:A:551:LEU:HD11	2.20	0.56
1:A:5:ILE:HD11	1:A:119:PRO:HD2	1.87	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:H5''	3:E:704:DG:N3	2.20	0.56
1:C:407:GLN:NE2	2:D:418:ASN:HA	2.20	0.56
1:C:23:GLN:NE2	1:C:60:VAL:HG12	2.18	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:473:THR:O	1:C:477:THR:HG23	2.06	0.55
1:C:75:VAL:HB	1:C:77:PHE:CE2	2.42	0.55
2:D:160:PHE:CD2	2:D:160:PHE:O	2.60	0.55
2:B:115:TYR:HD2	2:B:115:TYR:N	2.05	0.55
1:A:523:GLU:O	1:A:527:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:LEU:HB3	2:D:172:LYS:HE3	1.88	0.55
4:F:815:DG:H2'	4:F:815:DG:OP2	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: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
1:C:77:PHE:O	1:C:80:LEU:N	2.40	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
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: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:N	1:A:123:ASP:OD2	2.42	0.52
1:A:135:ILE:HG23	1:A:138:GLU:HB2	1.90	0.52
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:SER:O	2:B:190:GLY:HA2	2.09	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:A:101:LYS:HE2	1:A:321:PRO:HG3	1.91	0.52
1:C:199:ARG:HE	1:C:222:GLN:HG2	1.72	0.52
1:C:41:MET:HA	1:C:44:GLU:OE1	2.10	0.52
2:D:111:VAL:HG23	2:D:115:TYR:HE1	1.74	0.52
2:D:16:MET:CG	2:D:83:ARG:HG2	2.39	0.52
1:A:31:ILE:HG21	1:A:135:ILE:HA	1.90	0.52
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
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:HG22	2:D:419:THR:O	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
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:D:109:LEU:HD22	2:D:216:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:317:VAL:HG23	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
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:179:VAL:O	1:C:189:VAL:HA	2.12	0.50
1:C:94:ILE:HD11	3:E:708:DG:N2	2.26	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:184:MET:HG2	4:P:822:ATM:H1'	1.94	0.49
1:A:63:ILE:O	1:A:72:ARG:HB3	2.12	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:115:TYR:CD2	1:C:151:GLN:HG2	2.47	0.49
1:C:28:GLU:HB2	1:C:135:ILE:HG21	1.95	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:A:500:GLN:CD	2:B:422:LEU:HD11	2.32	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:130:PHE:H	1:A:130:PHE:HD2	1.59	0.49
1:A:97:PRO:HD3	1:A:232:TYR:CE2	2.47	0.49
2:B:118:VAL:HG12	2:B:119:PRO:O	2.12	0.49
2:B:69:THR:O	2:B:69:THR:HG22	2.12	0.49
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:A:2:ILE:CD1	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
2:D:360:ALA:C	2:D:362:THR:H	2.17	0.48
1:A:2:ILE:CD1	1:A:2:ILE:H	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:135:ILE:HG22	1:A:138:GLU:HB2	1.95	0.48
1:A:24:TRP:O	1:A:26:LEU:HG	2.14	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:HD2	1:C:130:PHE:H	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
2:B:124:PHE:HE2	2:B:153:TRP:CZ2	2.32	0.47
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.49	0.47
4:P:811:DG:H2''	4:P:812:DT:O5'	2.14	0.47
1:C:115:TYR:HD2	1:C:151:GLN:HG2	1.79	0.47
1:C:37:ILE:HA	1:C:40:GLU:HG3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.95	0.47
1:C:221:HIS:N	1:C:221:HIS:ND1	2.63	0.47
2:D:84:THR:O	2:D:84:THR:HG22	2.14	0.47
1:A:122:GLU:OE2	1:A:125:ARG:NH1	2.48	0.47
1:A:79:GLU:OE1	1:A:83:ARG:NH2	2.48	0.47
2:D:203:GLU:O	2:D:207:GLN:HG2	2.14	0.47
2:D:419:THR:O	2:D:420:PRO:C	2.50	0.47
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:A:226:PRO:HB3	1:A:235:HIS:CD2	2.50	0.47
2:B:164:MET:HE2	2:B:168:LEU:HD11	1.95	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:214:LEU:HD12	2:B:215:THR:H	1.80	0.47
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.45	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
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.97	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:114:ALA:HB1	1:A:160:PHE:CE2	2.50	0.46
1:A:35:VAL:HA	1:A:38:CYS:HB2	1.97	0.46
1:A:135:ILE:HG12	1:A:136:ASN:N	2.27	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:228:LEU:HD22	1:A:242:GLN:NE2	2.31	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:C:65:LYS:HE2	1:C:72:ARG:HD3	1.98	0.46
1:A:164:MET:HE2	1:A:168:LEU:HD11	1.96	0.46
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.30	0.46
1:A:88:TRP:CD1	2:B:143:ARG:NH1	2.84	0.46
1:C:120:LEU:HG	1:C:121:ASP:N	2.30	0.46
1:C:64:LYS:HD3	1:C:71:TRP:CE2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:88:TRP:CD1	2:D:143:ARG:NH1	2.83	0.46
1:A:186:ASP:CB	4:P:822:ATM:N5'	2.78	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
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.15	0.46
2:B:87:PHE:CD2	2:B:87:PHE:C	2.88	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:O	2:D:205:LEU:HD12	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:221:HIS:ND1	1:A:221:HIS:N	2.63	0.45
1:A:60:VAL:HG11	1:A:130:PHE:CD1	2.47	0.45
1:A:131:THR:HA	1:A:143:ARG:HG2	1.98	0.45
1:A:8:VAL:HG12	1:A:8:VAL:O	2.16	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: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: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:60:VAL:CG1	1:A:130:PHE:HD1	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:OG1	1:A:29:GLU:HB3	2.17	0.44
2:B:247:PRO:CA	2:B:428:GLN:HE22	2.30	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
2:D:13:LYS:HD3	2:D:85:GLN:HB3	1.98	0.44
1:C:120:LEU:HG	1:C:121:ASP:H	1.82	0.44
2:D:323:LYS:O	2:D:385:LYS:NZ	2.50	0.44
2:D:78:ARG:HD3	2:D:411:ILE:O	2.17	0.44
1:A:77:PHE:O	1:A:80:LEU:N	2.49	0.44
2:D:109:LEU:HA	2:D:109:LEU:HD23	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: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
2:D:81:ASN:HB3	2:D:154:LYS:HD2	2.00	0.44
3:E:712:DC:H2''	3:E:713:DC:O5'	2.18	0.44
4:P:818:DC:H2'	4:P:819:DG:H8	1.83	0.44
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.98	0.44
2:B:69:THR:CG2	2:B:69:THR:O	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:16:MET:CE	1:C:83:ARG:HG2	2.48	0.44
1:C:253:THR:HG22	1:C:292:VAL:CG1	2.39	0.44
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.53	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
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:C:254:VAL:HG21	1:C:286:THR:CG2	2.44	0.43
2:D:428:GLN:HA	2:D:428:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:HG3	4:P:819:DG:OP1	2.17	0.43
1:A:130:PHE:N	1:A:130:PHE:CD2	2.87	0.43
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:132:ILE:HB	1:C:142:ILE:HG22	2.00	0.43
1:C:1:PRO:HB2	1:C:2:ILE:H	1.59	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
1:A:475:GLN:NE2	1:A:475:GLN:H	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
1:A:74:LEU:HD22	3:T:705:DA:C2	2.54	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: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:230:MET:O	4:F:821:DC:H5'	2.18	0.42
1:C:31:ILE:CG2	1:C:134:SER:HA	2.50	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:134:SER:O	1:A:135:ILE:HB	2.19	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:OE1	2:D:207:GLN:HA	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
4:P:822:ATM:O5'	4:P:822:ATM:H6	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:270:ILE:HA	1:A:270:ILE:HD12	1.76	0.41
2:B:210:LEU:HA	2:B:214:LEU:O	2.20	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.41
2:B:428:GLN:HA	2:B:428:GLN:OE1	2.21	0.41
1:C:266:TRP:O	1:C:269:GLN:HG2	2.20	0.41
1:C:36:GLU:O	1:C:40:GLU:HG2	2.21	0.41
2:D:10:VAL:HG13	2:D:87:PHE:CD1	2.55	0.41
1:A:23:GLN:HB3	1:A:23:GLN:HE21	1.64	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:C:31:ILE:HG21	1:C:134:SER:HA	2.02	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
2:B:86:ASP:O	2:B:90:VAL:HB	2.21	0.41
1:C:60:VAL:HG11	1:C:130:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.21	0.41
2:B:382:ILE:HG22	2:B:383:TRP:CE2	2.56	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
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
1:A:28:GLU:CD	1:A:28:GLU:H	2.24	0.40
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.20	0.40
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.40
2:B:50:ILE:HG13	2:B:51:GLY:N	2.35	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
1:C:54:ASN:HA	1:C:55:PRO:HD2	1.86	0.40
2:D:422:LEU:HD12	2:D:422:LEU:HA	1.77	0.40
2:B:297:GLU:OE1	2:B:297:GLU:HA	2.21	0.40
2:B:53:GLU:HG2	2:B:54:ASN:N	2.35	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: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
1:A:553:SER:O	1:A:554:ALA:C	2.59	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:HB2	2:D:336:GLN:HE21	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:420:PRO:HA	1:C:421:PRO:C	2.40	0.40
1:C:382:ILE:O	2:D:136:ASN:HB2	2.21	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%)	47	73
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%)	51	78

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%)	476 (96%)	19 (4%)	33	62
1	C	495/497 (100%)	475 (96%)	20 (4%)	31	60
2	B	374/390 (96%)	362 (97%)	12 (3%)	39	68
2	D	374/390 (96%)	366 (98%)	8 (2%)	53	80
All	All	1738/1774 (98%)	1679 (97%)	59 (3%)	37	66

All (59) 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	23	GLN
1	A	39	THR
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	277	ARG
1	A	293	ILE
1	A	324	ASP
1	A	338	THR
1	A	523	GLU
2	B	72	ARG
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	257	ILE
2	B	293	ILE
2	B	336	GLN
2	B	422	LEU
1	C	2	ILE
1	C	3	SER
1	C	5	ILE
1	C	7	THR
1	C	48	SER
1	C	50	ILE
1	C	53	GLU
1	C	123	ASP
1	C	130	PHE
1	C	199	ARG
1	C	218	ASP
1	C	221	HIS

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Mol	Chain	Res	Type
1	C	250	ASP
1	C	270	ILE
1	C	324	ASP
1	C	338	THR
1	C	357	MET
1	C	407	GLN
1	C	459	THR
1	C	498	ASN
2	D	74	LEU
2	D	113	ASP
2	D	134	SER
2	D	248	GLU
2	D	336	GLN
2	D	379	SER
2	D	423	VAL
2	D	424	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	A	464	GLN
1	A	487	GLN
2	B	278	GLN
2	B	336	GLN
1	C	222	GLN
1	C	367	GLN
1	C	407	GLN
1	C	464	GLN
1	C	547	GLN
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	22,28,29	3.14	10 (45%)	23,39,42	1.82	6 (26%)
4	ATM	F	822	3,4	16,23,24	1.34	1 (6%)	17,32,35	1.69	3 (17%)
4	MRG	P	817	1,3,4	22,28,29	3.23	10 (45%)	23,39,42	1.91	7 (30%)
4	ATM	P	822	3,4	16,23,24	1.34	1 (6%)	17,32,35	2.28	4 (23%)

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	-	3/8/26/27	0/3/3/3
4	ATM	F	822	3,4	-	1/7/24/25	0/2/2/2
4	MRG	P	817	1,3,4	-	3/8/26/27	0/3/3/3
4	ATM	P	822	3,4	-	1/7/24/25	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	817	MRG	C2-N2	9.21	1.48	1.34
4	P	817	MRG	C2-N2	9.06	1.48	1.34
4	P	817	MRG	C4-N3	5.89	1.44	1.35
4	F	817	MRG	C4-N3	5.62	1.44	1.35
4	P	817	MRG	C6-N1	5.42	1.42	1.33
4	F	817	MRG	C6-N1	4.97	1.41	1.33
4	F	822	ATM	C4-N3	4.50	1.40	1.33
4	P	817	MRG	C6-C5	4.42	1.49	1.41
4	F	817	MRG	C6-C5	4.39	1.48	1.41
4	P	822	ATM	C4-N3	4.29	1.40	1.33
4	P	817	MRG	C2'-C3'	-3.44	1.43	1.52
4	F	817	MRG	C2'-C3'	-3.41	1.43	1.52
4	P	817	MRG	O3'-C3'	-3.36	1.36	1.43
4	P	817	MRG	C2-N1	2.97	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	817	MRG	C2-N3	2.93	1.43	1.34
4	P	817	MRG	C2-N3	2.85	1.43	1.34
4	F	817	MRG	O4'-C4'	-2.78	1.38	1.45
4	F	817	MRG	C2-N1	2.78	1.43	1.34
4	P	817	MRG	O4'-C4'	-2.72	1.38	1.45
4	P	817	MRG	O5'-C5'	-2.67	1.38	1.44
4	F	817	MRG	O5'-C5'	-2.65	1.38	1.44
4	F	817	MRG	O3'-C3'	-2.53	1.38	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	822	ATM	C2'-C1'-N1	-6.12	100.15	114.27
4	P	822	ATM	C4-N3-C2	5.08	119.43	115.14
4	F	822	ATM	C4-N3-C2	4.74	119.14	115.14
4	F	817	MRG	C2-N3-C4	4.03	119.85	115.28
4	P	817	MRG	N3-C2-N1	-3.92	120.03	126.23
4	F	817	MRG	N3-C2-N1	-3.85	120.14	126.23
4	P	817	MRG	C2-N3-C4	3.34	119.06	115.28
4	P	817	MRG	C5-C6-N1	-3.30	118.92	123.43
4	P	817	MRG	C6-N1-C2	3.18	120.87	115.18
4	F	822	ATM	C5-C6-N1	-3.07	118.88	122.19
4	P	817	MRG	C22-C21-N2	3.06	119.71	111.49
4	P	822	ATM	C5-C6-N1	-2.87	119.10	122.19
4	F	817	MRG	C6-N1-C2	2.69	119.99	115.18
4	F	817	MRG	C5-C6-N1	-2.68	119.77	123.43
4	P	822	ATM	C5'-C4'-C3'	-2.65	106.22	114.29
4	F	817	MRG	C22-C21-N2	2.59	118.46	111.49
4	F	817	MRG	C4-C5-N7	-2.37	106.93	109.40
4	F	822	ATM	C2'-C1'-N1	-2.28	109.01	114.27
4	P	817	MRG	O5'-C5'-C4'	2.20	116.47	108.99
4	P	817	MRG	C4-C5-N7	-2.07	107.25	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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	817	MRG	1	0
4	P	822	ATM	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	1.07	97 (17%) 1 1	36, 83, 138, 149	0
1	C	554/556 (99%)	1.02	90 (16%) 1 1	34, 81, 136, 148	0
2	B	412/428 (96%)	0.67	30 (7%) 15 13	34, 66, 118, 131	0
2	D	412/428 (96%)	0.76	41 (9%) 7 5	40, 69, 125, 132	0
3	E	24/27 (88%)	0.98	5 (20%) 1 0	67, 104, 156, 164	0
3	T	24/27 (88%)	1.22	5 (20%) 1 0	69, 106, 158, 161	0
4	F	18/21 (85%)	0.49	2 (11%) 5 4	60, 92, 141, 142	0
4	P	18/21 (85%)	0.47	2 (11%) 5 4	68, 90, 142, 144	0
All	All	2017/2064 (97%)	0.90	272 (13%) 3 2	34, 75, 133, 164	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	14.2
1	A	133	PRO	13.9
1	C	142	ILE	13.4
1	A	74	LEU	12.5
1	C	133	PRO	12.3
3	T	702	DT	12.2
1	A	131	THR	12.1
2	D	231	GLY	11.1
2	D	214	LEU	10.8
2	B	215	THR	9.9
1	A	140	PRO	9.2
1	A	135	ILE	8.9
1	A	128	THR	7.7
1	C	140	PRO	7.4
1	C	287	LYS	7.4
1	A	34	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
2	D	4	PRO	7.4
1	C	136	ASN	7.4
2	D	94	ILE	7.0
1	C	132	ILE	6.9
1	C	293	ILE	6.9
1	A	72	ARG	6.9
1	A	26	LEU	6.8
2	B	88	TRP	6.8
1	A	132	ILE	6.7
1	A	52	PRO	6.7
1	A	129	ALA	6.6
1	A	130	PHE	6.6
1	C	26	LEU	6.5
2	D	212	TRP	6.5
1	C	138	GLU	6.5
1	A	134	SER	6.5
1	A	141	GLY	6.4
1	A	136	ASN	6.4
2	B	212	TRP	6.2
1	A	61	PHE	6.2
1	C	135	ILE	6.1
1	C	134	SER	6.1
1	C	223	LYS	6.1
1	C	61	PHE	6.1
1	C	24	TRP	5.9
1	C	252	TRP	5.9
1	C	34	LEU	5.8
1	C	144	TYR	5.8
1	A	66	LYS	5.7
1	C	25	PRO	5.7
1	A	549	ASP	5.6
1	A	19	PRO	5.6
1	A	59	PRO	5.5
1	C	129	ALA	5.5
1	A	30	LYS	5.4
1	A	142	ILE	5.4
3	T	725	DG	5.4
1	A	144	TYR	5.3
1	C	74	LEU	5.3
1	C	30	LYS	5.2
1	A	50	ILE	5.1
1	A	127	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLN	5.0
1	A	145	GLN	5.0
1	C	28	GLU	5.0
1	C	139	THR	4.9
1	A	137	ASN	4.9
1	C	141	GLY	4.9
1	C	60	VAL	4.8
1	A	63	ILE	4.8
3	E	702	DT	4.7
1	A	289	LEU	4.7
2	D	5	ILE	4.7
1	C	554	ALA	4.6
1	A	21	VAL	4.6
2	D	95	PRO	4.6
3	T	703	DG	4.6
1	A	75	VAL	4.5
1	A	29	GLU	4.5
2	B	295	LEU	4.5
2	B	428	GLN	4.4
1	A	550	LYS	4.4
2	B	89	GLU	4.3
1	A	139	THR	4.3
1	C	254	VAL	4.3
1	C	71	TRP	4.2
1	A	286	THR	4.2
2	D	216	THR	4.2
1	A	70	LYS	4.1
1	A	285	GLY	4.1
1	C	296	THR	4.1
1	C	130	PHE	4.1
1	A	49	LYS	4.1
1	A	146	TYR	4.1
1	C	69	THR	4.0
1	A	68	SER	4.0
1	C	145	GLN	4.0
2	B	5	ILE	4.0
2	D	67	ASP	4.0
2	D	89	GLU	4.0
1	A	62	ALA	4.0
1	C	137	ASN	4.0
4	P	803	DC	4.0
2	D	232	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
3	T	704	DG	3.9
2	D	90	VAL	3.9
1	C	295	LEU	3.9
1	C	78	ARG	3.8
1	A	223	LYS	3.8
3	E	704	DG	3.8
1	C	27	THR	3.8
2	D	358	ARG	3.7
1	C	21	VAL	3.7
2	D	215	THR	3.7
1	A	23	GLN	3.7
3	E	725	DG	3.7
2	B	250	ASP	3.7
1	C	292	VAL	3.7
1	A	56	TYR	3.6
2	B	422	LEU	3.6
1	A	293	ILE	3.6
1	C	448	ARG	3.5
1	A	27	THR	3.5
2	B	232	TYR	3.5
2	D	357	MET	3.5
1	A	77	PHE	3.5
1	A	71	TRP	3.5
2	D	88	TRP	3.5
1	A	28	GLU	3.5
1	C	303	LEU	3.4
1	A	33	ALA	3.4
2	D	354	TYR	3.4
1	C	143	ARG	3.4
2	B	213	GLY	3.4
1	C	109	LEU	3.4
2	D	124	PHE	3.4
2	D	177	ASP	3.4
2	D	360	ALA	3.4
1	A	32	LYS	3.4
2	B	301	LEU	3.4
1	A	124	PHE	3.4
1	A	54	ASN	3.4
1	C	49	LYS	3.4
1	A	448	ARG	3.3
2	D	213	GLY	3.3
1	A	553	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	4	PRO	3.3
1	A	69	THR	3.3
2	D	92	LEU	3.3
1	C	257	ILE	3.3
1	A	287	LYS	3.3
1	C	198	HIS	3.2
1	C	58	THR	3.2
1	C	75	VAL	3.1
1	C	63	ILE	3.1
1	C	301	LEU	3.1
1	A	60	VAL	3.1
1	A	37	ILE	3.1
1	A	31	ILE	3.1
1	A	25	PRO	3.1
2	D	7	THR	3.1
2	D	168	LEU	3.1
1	A	67	ASP	3.0
1	A	73	LYS	3.0
2	B	92	LEU	3.0
2	B	209	LEU	3.0
1	A	288	ALA	3.0
1	C	22	LYS	3.0
1	A	24	TRP	3.0
2	D	66	LYS	2.9
2	D	178	ILE	2.9
4	F	804	DA	2.9
1	A	36	GLU	2.9
1	C	131	THR	2.9
4	F	803	DC	2.9
3	E	703	DG	2.9
1	C	247	PRO	2.9
1	A	551	LEU	2.8
1	C	66	LYS	2.8
2	D	8	VAL	2.8
2	B	204	GLU	2.8
1	A	39	THR	2.8
2	D	361	HIS	2.8
1	A	544	GLY	2.8
2	B	281	LYS	2.8
2	D	428	GLN	2.8
1	C	222	GLN	2.8
4	P	804	DA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	283	LEU	2.7
2	B	282	LEU	2.7
1	C	70	LYS	2.7
1	A	78	ARG	2.7
1	A	546	GLU	2.7
3	T	724	DT	2.7
1	C	37	ILE	2.7
1	C	246	LEU	2.7
1	C	128	THR	2.7
1	C	224	GLU	2.7
1	A	200	THR	2.7
2	B	284	ARG	2.6
2	B	87	PHE	2.6
1	C	553	SER	2.6
1	C	294	PRO	2.6
1	C	50	ILE	2.5
1	A	138	GLU	2.5
1	A	18	GLY	2.5
2	D	209	LEU	2.5
2	B	277	ARG	2.5
1	A	38	CYS	2.5
1	A	261	VAL	2.5
2	D	118	VAL	2.5
2	D	187	LEU	2.5
1	A	234	LEU	2.5
1	C	311	LYS	2.5
3	E	724	DT	2.5
2	B	211	ARG	2.5
1	C	312	GLU	2.4
1	C	281	LYS	2.4
1	C	226	PRO	2.4
1	C	19	PRO	2.4
1	A	105	SER	2.4
2	B	154	LYS	2.4
1	A	149	LEU	2.4
1	C	33	ALA	2.4
2	B	90	VAL	2.4
1	A	143	ARG	2.4
1	A	298	GLU	2.4
1	A	254	VAL	2.4
1	C	36	GLU	2.4
1	C	23	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	299	ALA	2.4
2	D	422	LEU	2.4
1	A	552	VAL	2.3
1	A	148	VAL	2.3
1	C	54	ASN	2.3
1	A	194	GLU	2.3
1	C	73	LYS	2.3
2	D	356	ARG	2.3
2	D	119	PRO	2.3
1	C	308	GLU	2.3
1	C	17	ASP	2.3
2	D	173	LYS	2.3
1	C	251	SER	2.3
1	C	280	SER	2.3
1	A	284	ARG	2.3
2	D	211	ARG	2.2
2	B	173	LYS	2.2
1	C	57	ASN	2.2
1	C	124	PHE	2.2
1	A	83	ARG	2.2
1	A	193	LEU	2.2
1	C	237	ASP	2.2
1	C	228	LEU	2.2
1	C	299	ALA	2.2
2	D	202	ILE	2.2
1	C	297	GLU	2.2
1	C	300	GLU	2.2
1	A	154	LYS	2.1
1	C	310	LEU	2.1
1	A	102	LYS	2.1
1	A	543	GLY	2.1
2	B	159	ILE	2.1
1	A	292	VAL	2.1
1	C	260	LEU	2.1
1	C	291	GLU	2.1
2	B	168	LEU	2.1
1	A	65	LYS	2.1
1	C	298	GLU	2.0
1	C	278	GLN	2.0
1	A	283	LEU	2.0
2	D	189	VAL	2.0
1	A	227	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	236	PRO	2.0
2	D	197	GLN	2.0
2	B	425	LEU	2.0
2	D	284	ARG	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	0.90	0.18	88,102,117,121	0
4	MRG	F	817	26/27	0.91	0.14	84,99,117,127	0
4	ATM	F	822	22/23	0.93	0.18	71,78,87,95	0
4	ATM	P	822	22/23	0.94	0.16	71,82,95,95	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.