



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:08 AM UTC

PDB ID : 1R0A / pdb_00001r0a
Title : Crystal structure of HIV-1 reverse transcriptase covalently tethered to DNA template-primer solved to 2.8 angstroms
Authors : Tuske, S.; Ding, J.; Arnold, E.
Deposited on : 2003-09-19
Resolution : 2.80 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

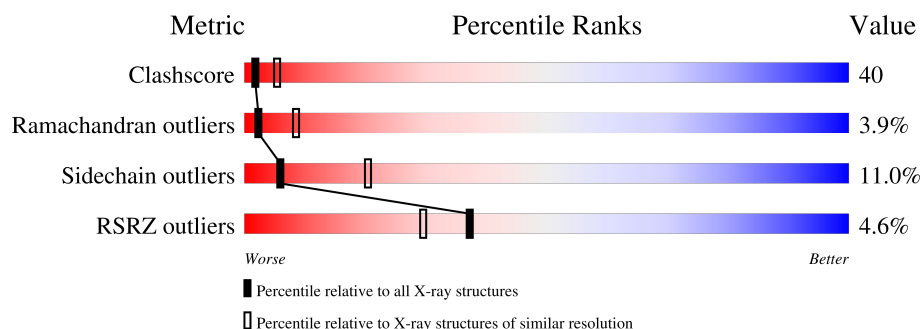
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	T	27	19% 63% 22% 11%
2	P	21	5% 14% 48% 33% 5%
3	A	558	6% 34% 52% 13%
4	B	429	5% 35% 53% 11%
5	L	211	33% 55% 11%
6	H	225	3% 50% 42% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	B	3001	-	X	-	-
7	GOL	P	3002	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12292 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 DNA chain called 5'-D(*A*TP*GP*CP*AP*TP*CP*GP*GP*CP*GP*CP*TP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*GP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	24	Total	C	N	O	P	0	0	0
			493	233	97	140	23			

- Molecule 2 is a DNA chain called 5'-D(*C*CP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*AP*GP*CP*GP*CP*CP*GP*(2DA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	20	Total	C	N	O	P	0	0	0
			402	192	72	119	19			

- Molecule 3 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	558	Total	C	N	O	S	15	0	0
			4482	2901	741	832	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 4 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	429	Total	C	N	O	S	4	0	0
			3534	2304	586	637	7			

There is a discrepancy between the modelled and reference sequences:

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

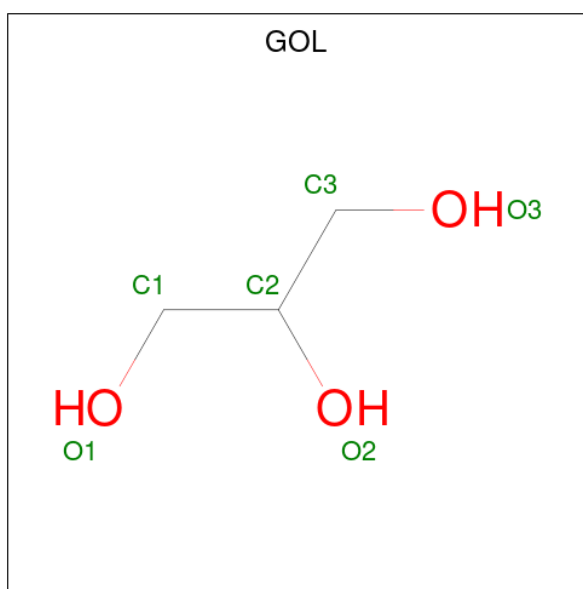
- Molecule 5 is a protein called monoclonal antibody (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	211	Total	C	N	O	S	0	0	0
			1643	1025	270	342	6			

- Molecule 6 is a protein called monoclonal antibody (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	225	Total	C	N	O	S	0	0	0
			1685	1060	276	340	9			

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

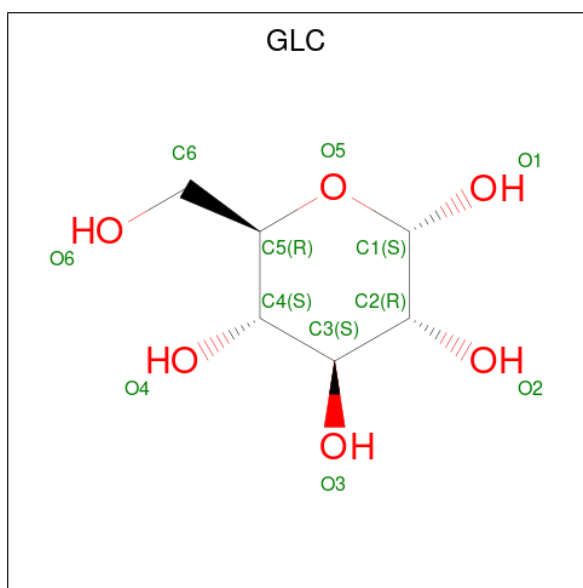


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	P	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	T	1	Total	O	0	0
			1	1		
10	A	7	Total	O	0	0
			7	7		
10	B	15	Total	O	0	0
			15	15		
10	L	2	Total	O	0	0
			2	2		
10	H	3	Total	O	0	0
			3	3		

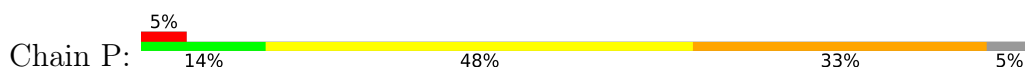
3 Residue-property plots [i](#)

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

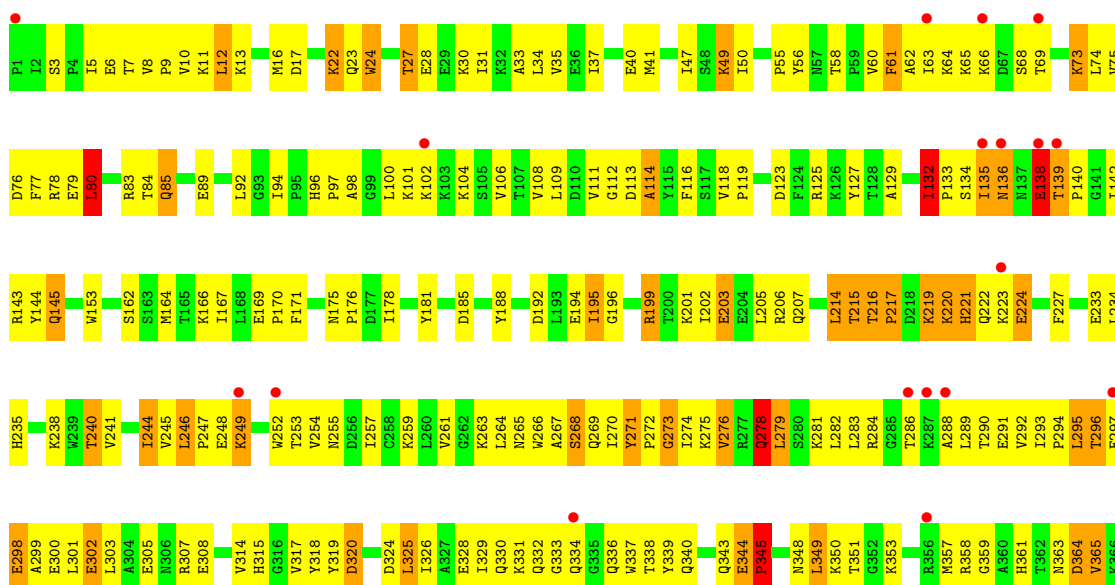
- Molecule 1: 5'-D(*A*TP*GP*CP*AP*TP*CP*GP*GP*CP*GP*CP*TP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*GP*GP*T)-3'

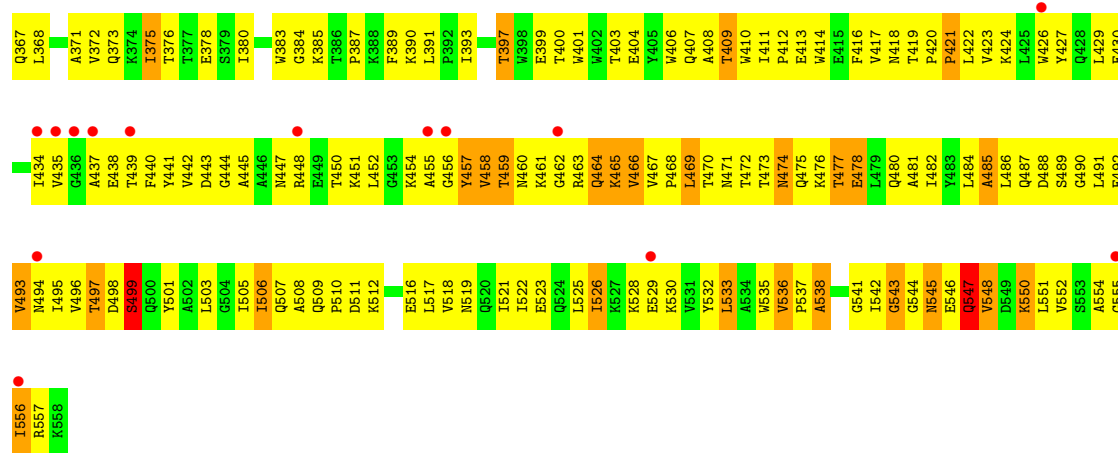


- Molecule 2: 5'-D(*C*CP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*AP*GP*CP*GP*CP*CP*GP*(2DA))-3'



- Molecule 3: Reverse transcriptase

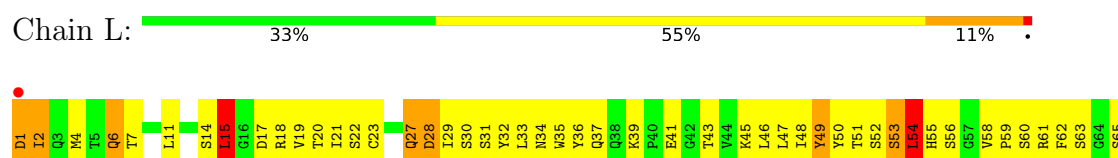


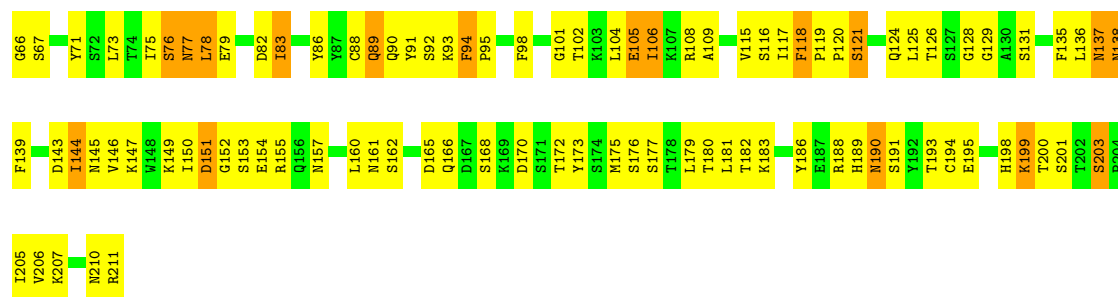


• Molecule 4: Reverse transcriptase

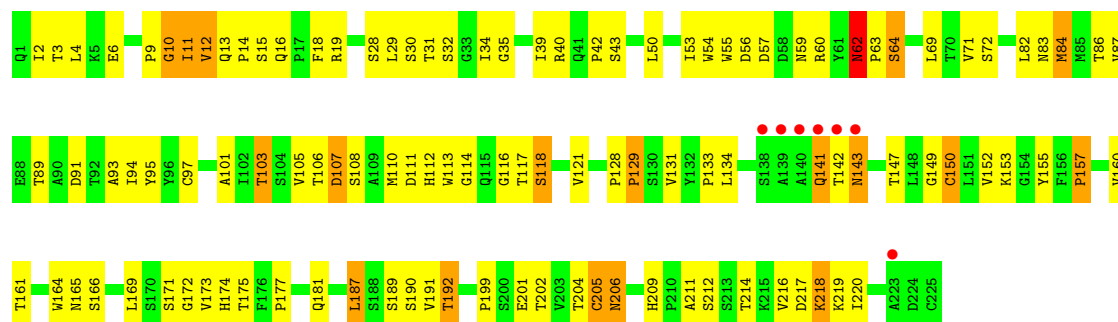


• Molecule 5: monoclonal antibody (light chain)





• Molecule 6: monoclonal antibody (heavy chain)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	165.82Å 165.82Å 220.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.96-2.80) 94.3 (19.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.239 , 0.272 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: GOL, GLC, 2DA, MG

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	T	0.49	0/554	1.14	7/854 (0.8%)
2	P	0.46	0/426	1.18	10/655 (1.5%)
3	A	0.64	0/4600	1.15	41/6259 (0.7%)
4	B	0.70	1/3639 (0.0%)	1.21	35/4949 (0.7%)
5	L	0.62	0/1681	1.14	15/2283 (0.7%)
6	H	0.67	0/1729	1.13	11/2372 (0.5%)
All	All	0.65	1/12629 (0.0%)	1.16	119/17372 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	B	0	2
5	L	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	16	MET	SD-CE	5.14	1.92	1.79

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	344	GLU	CA-C-N	11.33	134.00	119.84
3	A	344	GLU	C-N-CA	11.33	134.00	119.84
3	A	219	LYS	N-CA-C	-10.50	97.84	110.44
3	A	298	GLU	N-CA-C	-9.15	101.31	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	94	ILE	CA-C-N	9.11	129.18	119.89
4	B	94	ILE	C-N-CA	9.11	129.18	119.89
2	P	816	DG	N9-C1'-C2'	8.88	126.83	113.50
4	B	8	VAL	CA-C-N	8.75	128.51	119.76
4	B	8	VAL	C-N-CA	8.75	128.51	119.76
2	P	815	DA	N9-C1'-C2'	8.44	126.15	113.50
4	B	382	ILE	N-CA-C	8.41	119.21	110.72
1	T	711	DG	C2'-C3'-O3'	-8.12	99.31	111.50
5	L	137	ASN	N-CA-C	8.10	123.21	110.17
4	B	297	GLU	N-CA-C	-7.98	103.33	113.23
4	B	58	THR	CA-C-N	-7.88	112.58	120.31
4	B	58	THR	C-N-CA	-7.88	112.58	120.31
4	B	66	LYS	N-CA-C	-7.88	102.76	112.38
4	B	54	ASN	CA-C-N	7.88	129.69	119.84
4	B	54	ASN	C-N-CA	7.88	129.69	119.84
4	B	125	ARG	N-CA-C	7.85	120.74	111.71
2	P	815	DA	C2'-C3'-O3'	-7.54	100.20	111.50
3	A	320	ASP	CA-C-N	7.50	127.04	119.24
3	A	320	ASP	C-N-CA	7.50	127.04	119.24
1	T	713	DT	C2'-C3'-O3'	-7.50	100.25	111.50
6	H	111	ASP	N-CA-C	7.48	120.08	111.11
1	T	712	DC	C2'-C3'-O3'	-7.47	100.29	111.50
3	A	365	VAL	N-CA-C	-7.46	103.52	110.53
3	A	289	LEU	N-CA-C	7.37	126.50	110.80
4	B	147	ASN	N-CA-C	-7.33	104.95	114.04
3	A	249	LYS	N-CA-C	6.99	119.59	110.43
4	B	235	HIS	CA-C-N	6.83	128.38	119.84
4	B	235	HIS	C-N-CA	6.83	128.38	119.84
3	A	349	LEU	N-CA-C	-6.83	103.85	112.93
4	B	238	LYS	N-CA-C	-6.82	103.96	113.37
5	L	6	GLN	N-CA-C	-6.79	96.14	108.02
2	P	809	DT	C5'-C4'-C3'	-6.69	104.86	114.90
3	A	224	GLU	CA-C-N	-6.64	113.54	120.38
3	A	224	GLU	C-N-CA	-6.64	113.54	120.38
3	A	136	ASN	N-CA-C	6.64	117.23	108.07
4	B	390	LYS	N-CA-C	-6.54	96.49	107.99
3	A	125	ARG	N-CA-C	6.45	119.13	111.33
3	A	92	LEU	N-CA-C	6.30	120.97	113.16
4	B	289	LEU	N-CA-C	6.29	118.66	111.11
1	T	706	DT	N1-C1'-C2'	-6.26	104.11	113.50
4	B	115	TYR	N-CA-C	6.25	118.17	111.36
5	L	151	ASP	N-CA-C	-6.23	102.64	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	94	PHE	N-CA-C	-6.18	101.21	110.24
3	A	203	GLU	N-CA-C	-6.16	104.19	111.03
2	P	816	DG	C2'-C3'-O3'	-6.15	102.27	111.50
4	B	389	PHE	N-CA-C	6.13	118.72	108.73
3	A	138	GLU	N-CA-C	6.07	123.72	110.80
4	B	102	LYS	N-CA-C	6.07	120.52	113.18
5	L	168	SER	N-CA-C	6.05	117.95	111.36
3	A	80	LEU	N-CA-C	-6.03	104.63	111.14
4	B	427	TYR	N-CA-C	5.98	116.45	108.38
3	A	457	TYR	N-CA-C	5.97	119.25	110.59
3	A	345	PRO	N-CA-C	5.96	124.75	112.47
6	H	131	VAL	N-CA-C	5.96	116.89	108.36
4	B	87	PHE	N-CA-C	5.94	117.44	110.97
4	B	194	GLU	N-CA-C	-5.92	102.54	110.24
2	P	821	DG	C2'-C3'-O3'	-5.91	102.64	111.50
3	A	216	THR	CA-C-N	5.86	127.17	119.84
3	A	216	THR	C-N-CA	5.86	127.17	119.84
6	H	12	VAL	N-CA-C	5.86	116.55	108.12
6	H	97	CYS	N-CA-C	-5.86	100.25	109.50
3	A	557	ARG	N-CA-C	5.83	115.72	108.19
3	A	271	TYR	CA-C-N	5.75	127.02	119.84
3	A	271	TYR	C-N-CA	5.75	127.02	119.84
3	A	77	PHE	N-CA-C	5.74	119.81	113.21
2	P	820	DC	C2'-C3'-O3'	-5.73	102.90	111.50
5	L	66	GLY	N-CA-C	5.72	117.77	110.96
6	H	62	ASN	CA-C-N	5.72	126.99	119.84
6	H	62	ASN	C-N-CA	5.72	126.99	119.84
3	A	241	VAL	N-CA-C	-5.69	101.38	108.89
3	A	6	GLU	N-CA-C	-5.68	102.62	110.35
3	A	274	ILE	N-CA-C	-5.68	99.88	108.17
2	P	817	DC	C2'-C3'-O3'	-5.66	103.01	111.50
5	L	105	GLU	N-CA-C	5.63	119.38	109.80
4	B	343	GLN	N-CA-C	-5.63	106.46	113.55
5	L	176	SER	N-CA-C	-5.62	101.70	110.42
2	P	818	DG	C2'-C3'-O3'	-5.62	103.08	111.50
6	H	117	THR	N-CA-C	-5.62	99.15	108.75
1	T	710	DC	C2'-C3'-O3'	-5.59	103.11	111.50
3	A	132	ILE	CA-C-N	5.57	126.80	119.84
3	A	132	ILE	C-N-CA	5.57	126.80	119.84
4	B	85	GLN	N-CA-C	5.54	119.66	113.01
3	A	252	TRP	N-CA-C	5.52	117.34	107.80
5	L	67	SER	N-CA-C	5.52	116.92	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	391	LEU	N-CA-C	5.51	116.90	109.24
3	A	375	ILE	CB-CA-C	-5.50	104.84	112.04
5	L	186	TYR	N-CA-C	-5.50	105.20	111.14
4	B	354	TYR	N-CA-C	-5.46	101.56	109.59
5	L	54	LEU	N-CA-C	5.46	117.12	108.67
6	H	101	ALA	N-CA-C	5.42	118.24	108.48
3	A	426	TRP	N-CA-C	5.38	118.06	111.82
6	H	220	ILE	N-CA-C	5.35	111.94	106.21
4	B	291	GLU	N-CA-C	5.35	117.19	108.63
1	T	704	DC	O5'-P-OP1	-5.35	92.96	109.00
4	B	99	GLY	N-CA-C	5.33	120.32	114.40
4	B	132	ILE	CA-C-N	5.33	125.80	120.52
4	B	132	ILE	C-N-CA	5.33	125.80	120.52
3	A	106	VAL	N-CA-C	5.33	115.38	108.35
3	A	123	ASP	N-CA-C	5.30	119.00	112.54
5	L	15	LEU	N-CA-C	-5.28	103.37	110.24
5	L	2	ILE	N-CA-C	-5.26	99.90	107.37
3	A	499	SER	N-CA-C	5.17	116.95	108.52
3	A	12	LEU	N-CA-C	-5.16	102.42	110.42
3	A	506	ILE	N-CA-C	5.15	115.29	110.30
6	H	141	GLN	N-CA-C	5.14	116.92	110.24
3	A	493	VAL	N-CA-C	5.10	114.99	107.75
4	B	271	TYR	CA-C-N	5.10	126.21	119.84
4	B	271	TYR	C-N-CA	5.10	126.21	119.84
5	L	118	PHE	N-CA-C	5.10	117.56	109.40
3	A	487	GLN	N-CA-C	-5.08	105.93	112.68
1	T	708	DG	N9-C1'-C2'	-5.07	105.90	113.50
2	P	815	DA	C4'-C3'-O3'	-5.06	102.41	110.00
6	H	107	ASP	N-CA-C	5.04	116.96	109.25
4	B	73	LYS	N-CA-C	-5.03	103.41	110.50
5	L	30	SER	N-CA-C	5.00	118.11	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	188	TYR	Sidechain
4	B	405	TYR	Sidechain
5	L	49	TYR	Sidechain

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	T	493	0	269	38	0
2	P	402	0	226	23	0
3	A	4482	0	4485	420	0
4	B	3534	0	3568	282	2
5	L	1643	0	1565	141	0
6	H	1685	0	1640	99	0
7	B	6	0	4	0	0
7	P	6	0	4	0	0
8	A	1	0	0	0	0
9	H	12	0	12	2	0
10	A	7	0	0	1	0
10	B	15	0	0	0	0
10	H	3	0	0	1	0
10	L	2	0	0	0	0
10	T	1	0	0	0	0
All	All	12292	0	11773	959	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (959) 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:T:703:DG:H1'	1:T:704:DC:OP1	1.50	1.11
3:A:498:ASP:HB2	3:A:538:ALA:HB2	1.17	1.10
3:A:22:LYS:H	3:A:22:LYS:HD3	1.12	1.09
1:T:721:DG:H2''	1:T:722:DG:H5''	1.10	1.08
4:B:296:THR:HG22	4:B:298:GLU:H	1.09	1.07
3:A:246:LEU:HD23	3:A:246:LEU:H	1.17	1.07
4:B:261:VAL:HG13	4:B:276:VAL:HG11	1.37	1.06
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.36	1.05
3:A:104:LYS:HB2	3:A:192:ASP:HA	1.39	1.05
1:T:721:DG:C2'	1:T:722:DG:H5''	1.87	1.04
3:A:293:ILE:HD12	3:A:294:PRO:HD2	1.38	1.01
4:B:330:GLN:HE22	4:B:340:GLN:HE22	1.05	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.39	1.00
3:A:459:THR:HG23	3:A:463:ARG:HB3	1.44	1.00
1:T:703:DG:H1'	1:T:704:DC:P	2.01	0.99
3:A:5:ILE:HD11	3:A:167:ILE:HD11	1.45	0.98
5:L:4:MET:HE2	5:L:90:GLN:HB2	1.47	0.96
1:T:721:DG:H2''	1:T:722:DG:C5'	1.95	0.95
3:A:440:PHE:HE2	3:A:489:SER:HG	0.94	0.94
5:L:15:LEU:HD12	5:L:15:LEU:H	1.30	0.94
5:L:34:ASN:HD22	5:L:89:GLN:HE22	1.08	0.94
3:A:248:GLU:HB3	3:A:307:ARG:HH22	1.31	0.93
3:A:498:ASP:CB	3:A:538:ALA:HB2	1.99	0.92
6:H:165:ASN:HB2	6:H:169:LEU:HD13	1.51	0.92
4:B:260:LEU:HD21	4:B:303:LEU:HD13	1.52	0.92
5:L:90:GLN:HE21	5:L:92:SER:H	1.09	0.92
4:B:330:GLN:HE22	4:B:340:GLN:NE2	1.69	0.90
5:L:146:VAL:HG21	5:L:175:MET:HE1	1.49	0.90
3:A:278:GLN:HG3	3:A:302:GLU:CB	2.02	0.90
3:A:111:VAL:HG11	3:A:214:LEU:HD12	1.54	0.90
3:A:406:TRP:HE1	4:B:418:ASN:ND2	1.69	0.89
4:B:135:ILE:HD12	4:B:135:ILE:O	1.73	0.89
2:P:807:DC:H4'	3:A:448:ARG:HD2	1.55	0.89
3:A:550:LYS:HE2	3:A:550:LYS:HA	1.55	0.88
3:A:3:SER:OG	3:A:5:ILE:HG13	1.74	0.87
4:B:296:THR:HG22	4:B:298:GLU:N	1.90	0.87
5:L:61:ARG:HB2	5:L:76:SER:HB3	1.56	0.87
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.10	0.86
3:A:253:THR:HA	3:A:292:VAL:HA	1.58	0.86
3:A:435:VAL:HG22	4:B:290:THR:CG2	2.06	0.85
1:T:713:DT:H2''	1:T:714:DC:H5'	1.59	0.85
3:A:296:THR:HG22	3:A:298:GLU:H	1.41	0.84
4:B:222:GLN:HG3	4:B:224:GLU:H	1.40	0.84
3:A:420:PRO:HG3	3:A:422:LEU:HG	1.56	0.84
5:L:195:GLU:HG2	5:L:206:VAL:HG22	1.59	0.84
4:B:257:ILE:O	4:B:261:VAL:HG23	1.79	0.83
6:H:84:MET:HG2	6:H:87:VAL:HG12	1.59	0.83
3:A:24:TRP:HZ3	3:A:61:PHE:HB3	1.44	0.83
3:A:233:GLU:HB2	3:A:240:THR:HG23	1.58	0.83
3:A:246:LEU:H	3:A:246:LEU:CD2	1.91	0.83
2:P:809:DT:H2''	2:P:810:DG:C8	2.14	0.82
3:A:34:LEU:HD21	3:A:62:ALA:HB2	1.58	0.82
4:B:61:PHE:CZ	4:B:74:LEU:HD23	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:266:TRP:HH2	4:B:422:LEU:HD22	1.46	0.81
6:H:141:GLN:OE1	6:H:199:PRO:HD3	1.80	0.81
6:H:62:ASN:C	6:H:62:ASN:HD22	1.89	0.80
4:B:332:GLN:HG2	4:B:427:TYR:CD1	2.16	0.80
5:L:147:LYS:NZ	5:L:149:LYS:HD2	1.96	0.80
4:B:175:ASN:N	4:B:176:PRO:HD3	1.97	0.80
3:A:13:LYS:HB2	3:A:16:MET:HE3	1.63	0.80
3:A:450:THR:O	3:A:451:LYS:HG2	1.80	0.80
3:A:406:TRP:HE1	4:B:418:ASN:HD21	1.27	0.80
3:A:303:LEU:O	3:A:307:ARG:HG3	1.82	0.79
4:B:106:VAL:HG13	4:B:234:LEU:HB2	1.65	0.79
5:L:155:ARG:HE	5:L:157:ASN:HB2	1.45	0.79
3:A:199:ARG:NH2	3:A:220:LYS:HE2	1.98	0.79
3:A:498:ASP:HB2	3:A:538:ALA:CB	2.09	0.79
5:L:90:GLN:HE21	5:L:92:SER:N	1.80	0.79
2:P:818:DG:H2'	2:P:819:DC:C6	2.19	0.78
3:A:466:VAL:HG21	3:A:551:LEU:HG	1.63	0.78
3:A:463:ARG:C	3:A:464:GLN:HE21	1.91	0.77
3:A:439:THR:HG21	4:B:289:LEU:H	1.49	0.77
3:A:317:VAL:HG22	3:A:318:TYR:N	2.00	0.76
3:A:466:VAL:HG12	3:A:466:VAL:O	1.84	0.76
4:B:261:VAL:HG13	4:B:276:VAL:CG1	2.13	0.76
3:A:443:ASP:O	3:A:481:ALA:HB2	1.85	0.76
4:B:356:ARG:HE	4:B:360:ALA:CB	1.97	0.76
3:A:23:GLN:HE22	3:A:60:VAL:H	1.31	0.76
4:B:237:ASP:C	4:B:239:TRP:H	1.93	0.76
3:A:73:LYS:HZ2	3:A:73:LYS:HB3	1.50	0.76
4:B:8:VAL:HG11	4:B:159:ILE:HG12	1.68	0.76
3:A:465:LYS:O	3:A:466:VAL:HG23	1.86	0.76
1:T:703:DG:C1'	1:T:704:DC:OP1	2.33	0.76
1:T:722:DG:H2''	1:T:723:DA:H5'	1.68	0.75
6:H:10:GLY:HA2	6:H:118:SER:O	1.87	0.75
3:A:420:PRO:HA	3:A:422:LEU:N	2.01	0.75
3:A:430:GLU:HB2	3:A:532:TYR:HB2	1.67	0.75
4:B:238:LYS:O	4:B:238:LYS:HD3	1.85	0.75
4:B:34:LEU:HD11	4:B:73:LYS:HG3	1.69	0.75
3:A:517:LEU:O	3:A:521:ILE:HG13	1.87	0.75
3:A:400:THR:O	3:A:403:THR:HG22	1.87	0.75
4:B:387:PRO:HG2	4:B:389:PHE:CE1	2.21	0.75
6:H:53:ILE:HB	6:H:71:VAL:CG1	2.16	0.74
6:H:103:THR:HG21	9:H:1725:GLC:H4	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:253:THR:O	4:B:257:ILE:HG12	1.87	0.74
4:B:317:VAL:HG12	4:B:349:LEU:HD23	1.68	0.74
3:A:478:GLU:OE1	3:A:498:ASP:OD1	2.05	0.74
3:A:460:ASN:ND2	4:B:288:ALA:HB2	2.03	0.74
3:A:253:THR:HG22	3:A:292:VAL:HG22	1.69	0.73
3:A:297:GLU:HA	3:A:300:GLU:HB2	1.70	0.73
4:B:363:ASN:C	4:B:363:ASN:HD22	1.95	0.73
4:B:266:TRP:CH2	4:B:422:LEU:HD22	2.22	0.73
6:H:160:VAL:HG21	6:H:187:LEU:HD11	1.68	0.73
3:A:533:LEU:HD12	3:A:533:LEU:N	2.02	0.73
3:A:555:GLY:O	3:A:556:ILE:HG13	1.88	0.73
4:B:254:VAL:HB	4:B:289:LEU:O	1.88	0.73
3:A:317:VAL:HG22	3:A:318:TYR:H	1.53	0.73
3:A:473:THR:O	3:A:476:LYS:N	2.21	0.73
3:A:491:LEU:HD23	3:A:529:GLU:OE2	1.88	0.73
4:B:356:ARG:HE	4:B:360:ALA:HB3	1.54	0.73
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.70	0.73
3:A:61:PHE:H	3:A:61:PHE:HD2	1.37	0.72
4:B:60:VAL:CG1	4:B:75:VAL:HG22	2.17	0.72
5:L:146:VAL:CG2	5:L:175:MET:HE1	2.19	0.72
4:B:112:GLY:HA3	4:B:151:GLN:HE21	1.52	0.72
6:H:19:ARG:NH1	6:H:83:ASN:HD21	1.86	0.72
3:A:494:ASN:HB3	4:B:289:LEU:HD12	1.71	0.72
5:L:151:ASP:HA	5:L:191:SER:HB3	1.71	0.72
6:H:62:ASN:HD22	6:H:63:PRO:N	1.88	0.72
4:B:46:LYS:HD2	4:B:148:VAL:HG21	1.72	0.72
3:A:266:TRP:O	3:A:269:GLN:HG2	1.90	0.71
4:B:79:GLU:OE1	4:B:83:ARG:NH1	2.22	0.71
1:T:702:DT:H4'	1:T:703:DG:OP2	1.90	0.71
1:T:713:DT:H2'	1:T:714:DC:C6	2.24	0.71
3:A:419:THR:H	3:A:422:LEU:HD21	1.55	0.71
1:T:713:DT:H2'	1:T:714:DC:H6	1.56	0.71
5:L:17:ASP:O	5:L:77:ASN:HA	1.91	0.71
3:A:64:LYS:HE2	3:A:66:LYS:NZ	2.06	0.71
5:L:34:ASN:OD1	5:L:49:TYR:HA	1.91	0.71
3:A:22:LYS:HD3	3:A:22:LYS:N	1.97	0.71
3:A:73:LYS:HB3	3:A:73:LYS:NZ	2.05	0.71
3:A:447:ASN:ND2	3:A:450:THR:HG23	2.06	0.70
3:A:175:ASN:HB3	3:A:178:ILE:HD12	1.72	0.70
3:A:275:LYS:HE3	3:A:332:GLN:OE1	1.91	0.70
6:H:18:PHE:CD2	6:H:87:VAL:HG11	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:279:LEU:CD2	3:A:279:LEU:H	2.05	0.70
3:A:320:ASP:H	3:A:343:GLN:HE22	1.38	0.70
4:B:260:LEU:HG	4:B:264:LEU:HD12	1.72	0.70
3:A:7:THR:HG22	3:A:119:PRO:HB2	1.72	0.70
4:B:103:LYS:HE3	4:B:103:LYS:HA	1.74	0.69
3:A:37:ILE:HG22	3:A:41:MET:HE2	1.73	0.69
1:T:703:DG:C1'	1:T:704:DC:P	2.80	0.69
4:B:175:ASN:H	4:B:176:PRO:HD3	1.56	0.69
5:L:105:GLU:OE2	5:L:173:TYR:OH	2.10	0.69
3:A:444:GLY:HA2	3:A:552:VAL:HG11	1.73	0.69
4:B:365:VAL:O	4:B:369:THR:HG23	1.92	0.69
3:A:13:LYS:HD2	3:A:16:MET:HE1	1.75	0.69
3:A:139:THR:HG22	3:A:140:PRO:O	1.92	0.69
3:A:522:ILE:O	3:A:526:ILE:HG22	1.91	0.69
3:A:217:PRO:HB2	3:A:219:LYS:HG2	1.75	0.69
5:L:146:VAL:HG21	5:L:175:MET:CE	2.22	0.69
3:A:350:LYS:NZ	3:A:378:GLU:OE1	2.27	0.68
3:A:454:LYS:NZ	3:A:554:ALA:HB3	2.08	0.68
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.74	0.68
6:H:3:THR:C	6:H:4:LEU:HD12	2.19	0.68
4:B:292:VAL:HG12	4:B:292:VAL:O	1.93	0.68
3:A:456:GLY:O	3:A:548:VAL:HG12	1.94	0.68
1:T:704:DC:H4'	1:T:705:DA:H5'	1.76	0.68
3:A:547:GLN:N	3:A:547:GLN:HE21	1.92	0.68
3:A:96:HIS:HD1	3:A:98:ALA:H	1.40	0.67
5:L:31:SER:O	5:L:50:TYR:HD1	1.76	0.67
3:A:22:LYS:H	3:A:22:LYS:CD	1.96	0.67
5:L:34:ASN:HB2	5:L:89:GLN:NE2	2.09	0.67
3:A:278:GLN:HE21	3:A:302:GLU:HA	1.59	0.67
3:A:368:LEU:O	3:A:372:VAL:HG23	1.94	0.67
6:H:62:ASN:C	6:H:62:ASN:ND2	2.49	0.67
3:A:261:VAL:HG23	3:A:276:VAL:HG11	1.76	0.67
4:B:229:TRP:HA	4:B:232:TYR:CE1	2.30	0.67
3:A:49:LYS:HB2	3:A:49:LYS:NZ	2.10	0.66
4:B:12:LEU:HD23	4:B:84:THR:HG22	1.76	0.66
3:A:246:LEU:HD23	3:A:246:LEU:N	2.00	0.66
1:T:715:DG:H1'	1:T:716:DA:C8	2.29	0.66
3:A:440:PHE:CZ	3:A:488:ASP:O	2.48	0.66
4:B:195:ILE:HG12	4:B:199:ARG:NE	2.10	0.66
3:A:35:VAL:CG2	3:A:132:ILE:HD11	2.24	0.66
4:B:242:GLN:OE1	4:B:353:LYS:HD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:11:LYS:O	3:A:85:GLN:HG2	1.95	0.66
3:A:438:GLU:OE2	3:A:463:ARG:NH2	2.28	0.66
3:A:397:THR:HG21	3:A:424:LYS:HA	1.78	0.66
1:T:716:DA:H2''	1:T:717:DA:H5'	1.78	0.66
3:A:139:THR:HG23	3:A:140:PRO:HD2	1.78	0.66
3:A:463:ARG:HG3	3:A:464:GLN:N	2.09	0.66
1:T:704:DC:O2	1:T:704:DC:C2'	2.43	0.66
3:A:447:ASN:HD22	3:A:450:THR:HG23	1.58	0.66
4:B:220:LYS:NZ	4:B:222:GLN:HB2	2.11	0.66
3:A:222:GLN:O	3:A:224:GLU:HG3	1.95	0.65
4:B:366:LYS:O	4:B:370:GLU:HG3	1.97	0.65
5:L:137:ASN:HB3	5:L:138:ASN:HD22	1.61	0.65
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.31	0.65
3:A:293:ILE:CD1	3:A:294:PRO:HD2	2.22	0.65
6:H:157:PRO:HD2	6:H:211:ALA:CB	2.27	0.65
5:L:18:ARG:HA	5:L:76:SER:O	1.97	0.65
3:A:104:LYS:HB2	3:A:192:ASP:CA	2.23	0.65
3:A:296:THR:HG22	3:A:298:GLU:N	2.09	0.65
3:A:219:LYS:O	3:A:219:LYS:HG3	1.97	0.65
4:B:98:ALA:O	4:B:101:LYS:HG2	1.96	0.65
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.32	0.64
2:P:812:DT:H6	3:A:358:ARG:HH12	1.45	0.64
3:A:34:LEU:CD2	3:A:62:ALA:HB2	2.28	0.64
5:L:23:CYS:SG	5:L:33:LEU:HD11	2.37	0.64
3:A:445:ALA:O	3:A:477:THR:HG21	1.97	0.64
3:A:485:ALA:O	3:A:489:SER:HB2	1.97	0.64
3:A:407:GLN:HG3	4:B:393:ILE:HA	1.80	0.64
3:A:458:VAL:HG12	3:A:458:VAL:O	1.97	0.64
4:B:427:TYR:CG	4:B:428:GLN:N	2.66	0.64
3:A:361:HIS:NE2	3:A:505:ILE:HD13	2.13	0.64
5:L:199:LYS:HG3	5:L:199:LYS:O	1.98	0.64
1:T:713:DT:H2''	1:T:714:DC:C5'	2.27	0.63
3:A:501:TYR:O	3:A:505:ILE:HG13	1.98	0.63
3:A:33:ALA:O	3:A:37:ILE:HG13	1.98	0.63
3:A:473:THR:O	3:A:474:ASN:C	2.41	0.63
4:B:175:ASN:N	4:B:176:PRO:CD	2.61	0.63
4:B:220:LYS:HZ3	4:B:222:GLN:HB2	1.63	0.63
6:H:204:THR:HG23	6:H:218:LYS:C	2.24	0.63
6:H:53:ILE:HB	6:H:71:VAL:HG12	1.79	0.63
3:A:265:ASN:HA	3:A:268:SER:OG	1.99	0.63
3:A:13:LYS:CB	3:A:16:MET:HE3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:THR:HG23	3:A:404:GLU:HG2	1.81	0.63
6:H:53:ILE:HB	6:H:71:VAL:HG11	1.79	0.63
3:A:24:TRP:CZ3	3:A:61:PHE:HB3	2.32	0.63
4:B:363:ASN:ND2	4:B:366:LYS:H	1.97	0.62
3:A:438:GLU:CD	3:A:463:ARG:HH21	2.07	0.62
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.63	0.62
3:A:270:ILE:HD11	3:A:315:HIS:O	1.99	0.62
6:H:13:GLN:HB2	6:H:16:GLN:HG3	1.80	0.62
2:P:805:DT:H4'	2:P:805:DT:OP1	1.99	0.62
3:A:199:ARG:HH22	3:A:220:LYS:HE2	1.65	0.62
3:A:203:GLU:HG3	3:A:207:GLN:HE21	1.64	0.62
3:A:288:ALA:O	3:A:291:GLU:HB3	1.99	0.62
5:L:46:LEU:HD23	5:L:55:HIS:CG	2.35	0.62
1:T:720:DG:H4'	1:T:720:DG:OP1	1.99	0.62
2:P:809:DT:C2'	2:P:810:DG:C8	2.82	0.62
4:B:104:LYS:NZ	4:B:104:LYS:HB3	2.14	0.62
4:B:175:ASN:HD21	4:B:201:LYS:NZ	1.97	0.62
3:A:28:GLU:HG3	3:A:135:ILE:HG13	1.82	0.62
3:A:338:THR:HG22	3:A:339:TYR:N	2.14	0.62
6:H:192:THR:O	6:H:192:THR:HG22	1.98	0.62
3:A:248:GLU:HB3	3:A:307:ARG:NH2	2.11	0.61
4:B:210:LEU:C	4:B:212:TRP:H	2.07	0.61
2:P:818:DG:H2'	2:P:819:DC:H6	1.63	0.61
4:B:116:PHE:O	4:B:148:VAL:HG11	2.01	0.61
6:H:32:SER:HA	6:H:55:TRP:CD1	2.35	0.61
3:A:460:ASN:HA	4:B:286:THR:O	1.99	0.61
4:B:246:LEU:HG	4:B:310:LEU:HD12	1.81	0.61
2:P:808:DC:H2''	2:P:809:DT:O5'	1.99	0.61
3:A:473:THR:O	3:A:475:GLN:N	2.34	0.61
3:A:220:LYS:HD3	3:A:220:LYS:C	2.25	0.61
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.23	0.61
3:A:202:ILE:O	3:A:206:ARG:HG3	2.00	0.61
3:A:325:LEU:HD21	3:A:383:TRP:CE3	2.36	0.61
5:L:106:ILE:HG13	5:L:166:GLN:OE1	1.99	0.61
3:A:143:ARG:HG3	3:A:143:ARG:HH11	1.63	0.61
3:A:469:LEU:HD21	3:A:480:GLN:HG2	1.81	0.61
3:A:529:GLU:O	3:A:530:LYS:HG3	2.01	0.61
4:B:101:LYS:O	4:B:236:PRO:HB2	2.00	0.61
5:L:15:LEU:H	5:L:15:LEU:CD1	2.08	0.61
3:A:61:PHE:HD2	3:A:61:PHE:N	1.98	0.61
4:B:206:ARG:HD2	4:B:216:THR:OG1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:34:ASN:ND2	5:L:89:GLN:HE22	1.90	0.61
4:B:199:ARG:NH2	4:B:230:MET:HE3	2.16	0.60
4:B:237:ASP:C	4:B:239:TRP:N	2.59	0.60
5:L:6:GLN:OE1	5:L:101:GLY:N	2.34	0.60
5:L:193:THR:HG23	5:L:206:VAL:HG13	1.83	0.60
4:B:97:PRO:HD3	4:B:181:TYR:CD1	2.36	0.60
4:B:393:ILE:HD11	4:B:397:THR:HG22	1.82	0.60
5:L:31:SER:O	5:L:50:TYR:CD1	2.54	0.60
3:A:478:GLU:OE1	3:A:498:ASP:CG	2.43	0.60
3:A:447:ASN:HD22	3:A:450:THR:CG2	2.14	0.60
4:B:326:ILE:HG21	4:B:390:LYS:HE2	1.82	0.60
6:H:166:SER:H	6:H:206:ASN:HD21	1.47	0.60
6:H:202:THR:HB	6:H:219:LYS:HE3	1.83	0.60
3:A:61:PHE:N	3:A:61:PHE:CD2	2.69	0.60
3:A:503:LEU:CD2	3:A:535:TRP:HB2	2.31	0.60
6:H:69:LEU:CD2	6:H:84:MET:HE3	2.32	0.60
3:A:64:LYS:HE2	3:A:66:LYS:HZ1	1.65	0.60
3:A:365:VAL:HG11	3:A:401:TRP:CD1	2.36	0.60
4:B:50:ILE:HG21	4:B:145:GLN:HG2	1.84	0.60
4:B:279:LEU:HD12	4:B:279:LEU:N	2.17	0.60
2:P:811:DT:OP2	3:A:359:GLY:HA2	2.00	0.60
3:A:246:LEU:CD2	3:A:246:LEU:N	2.61	0.60
3:A:279:LEU:H	3:A:279:LEU:HD23	1.67	0.59
4:B:114:ALA:HB1	4:B:160:PHE:CZ	2.37	0.59
5:L:137:ASN:HB3	5:L:138:ASN:ND2	2.17	0.59
4:B:279:LEU:HD12	4:B:279:LEU:H	1.66	0.59
6:H:3:THR:O	6:H:4:LEU:HD12	2.01	0.59
1:T:721:DG:C3'	1:T:722:DG:H5''	2.31	0.59
3:A:35:VAL:HG22	3:A:132:ILE:HD11	1.82	0.59
3:A:41:MET:HE1	3:A:73:LYS:CE	2.32	0.59
2:P:805:DT:H2'	2:P:806:DC:C6	2.38	0.59
3:A:17:ASP:O	3:A:83:ARG:NH1	2.35	0.59
3:A:365:VAL:HG11	3:A:401:TRP:CG	2.37	0.59
3:A:399:GLU:O	3:A:403:THR:HB	2.02	0.59
6:H:6:GLU:OE1	6:H:116:GLY:N	2.33	0.59
3:A:194:GLU:O	3:A:196:GLY:N	2.36	0.59
3:A:443:ASP:OD1	3:A:478:GLU:OE1	2.19	0.59
4:B:175:ASN:O	4:B:177:ASP:N	2.35	0.59
4:B:199:ARG:HH22	4:B:230:MET:HE3	1.68	0.59
5:L:144:ILE:HG23	5:L:145:ASN:N	2.18	0.59
6:H:18:PHE:HD2	6:H:87:VAL:HG11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:272:PRO:O	3:A:273:GLY:O	2.21	0.59
3:A:279:LEU:HD23	3:A:279:LEU:N	2.18	0.59
4:B:320:ASP:OD2	4:B:323:LYS:HG3	2.01	0.59
3:A:463:ARG:HG3	3:A:464:GLN:H	1.68	0.59
3:A:498:ASP:HA	3:A:536:VAL:O	2.03	0.59
4:B:175:ASN:C	4:B:177:ASP:H	2.11	0.59
5:L:48:ILE:HD12	5:L:73:LEU:HD13	1.85	0.59
3:A:455:ALA:HB2	3:A:477:THR:HB	1.84	0.59
4:B:223:LYS:HZ1	6:H:56:ASP:CG	2.10	0.59
5:L:106:ILE:H	5:L:166:GLN:HE22	1.50	0.59
3:A:11:LYS:H	3:A:85:GLN:HE21	1.51	0.59
3:A:361:HIS:CD2	3:A:505:ILE:HD13	2.38	0.59
3:A:371:ALA:O	3:A:375:ILE:HG12	2.03	0.59
6:H:19:ARG:HH12	6:H:83:ASN:HD21	1.51	0.59
4:B:262:GLY:O	4:B:265:ASN:HB3	2.02	0.58
4:B:2:ILE:HD12	4:B:2:ILE:H	1.67	0.58
4:B:8:VAL:CG1	4:B:159:ILE:HG12	2.33	0.58
1:T:723:DA:H2"	1:T:724:DC:OP2	2.02	0.58
4:B:344:GLU:HA	4:B:344:GLU:OE2	2.02	0.58
3:A:50:ILE:CG2	3:A:145:GLN:HB3	2.34	0.58
3:A:451:LYS:O	3:A:471:ASN:N	2.36	0.58
3:A:463:ARG:O	3:A:464:GLN:NE2	2.36	0.58
5:L:179:LEU:HG	5:L:181:LEU:HD21	1.84	0.58
6:H:128:PRO:HA	6:H:209:HIS:HD2	1.67	0.58
3:A:452:LEU:HB3	3:A:470:THR:HA	1.84	0.58
4:B:106:VAL:HG13	4:B:234:LEU:CB	2.33	0.58
3:A:244:ILE:HD13	3:A:267:ALA:HB2	1.86	0.58
3:A:279:LEU:HD22	3:A:302:GLU:CB	2.33	0.58
3:A:458:VAL:HG11	3:A:547:GLN:HB3	1.85	0.58
4:B:239:TRP:CH2	4:B:378:GLU:HA	2.38	0.58
3:A:326:ILE:HG21	3:A:390:LYS:HE2	1.86	0.58
3:A:317:VAL:CG2	3:A:318:TYR:H	2.16	0.58
3:A:441:TYR:CD2	3:A:544:GLY:CA	2.86	0.58
6:H:165:ASN:HD22	6:H:169:LEU:HD11	1.69	0.58
3:A:441:TYR:CD2	3:A:544:GLY:C	2.82	0.58
4:B:330:GLN:NE2	4:B:340:GLN:OE1	2.37	0.58
3:A:30:LYS:O	3:A:33:ALA:HB3	2.04	0.57
3:A:132:ILE:O	3:A:132:ILE:HG12	2.03	0.57
3:A:317:VAL:CG2	3:A:318:TYR:N	2.68	0.57
3:A:434:ILE:HG22	3:A:494:ASN:HD21	1.67	0.57
4:B:104:LYS:HG2	4:B:192:ASP:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:138:ASN:ND2	6:H:174:HIS:HE1	2.02	0.57
3:A:79:GLU:O	3:A:83:ARG:HD2	2.05	0.57
3:A:254:VAL:HG13	3:A:255:ASN:N	2.18	0.57
4:B:342:TYR:HB3	4:B:348:ASN:HA	1.87	0.57
5:L:136:LEU:HD23	5:L:144:ILE:HD13	1.86	0.57
5:L:146:VAL:HG12	5:L:147:LYS:N	2.19	0.57
3:A:56:TYR:O	3:A:143:ARG:NH2	2.37	0.57
6:H:89:THR:HA	6:H:121:VAL:HB	1.86	0.57
4:B:285:GLY:H	4:B:287:LYS:NZ	2.02	0.57
5:L:162:SER:OG	6:H:177:PRO:HG2	2.05	0.57
4:B:169:GLU:HB3	4:B:170:PRO:HD3	1.84	0.57
4:B:360:ALA:HB1	4:B:367:GLN:NE2	2.20	0.57
6:H:133:PRO:O	6:H:134:LEU:HD23	2.05	0.57
3:A:434:ILE:CG2	3:A:494:ASN:HD21	2.18	0.57
1:T:724:DC:H2''	1:T:725:DG:H8	1.70	0.56
3:A:220:LYS:HD3	3:A:220:LYS:O	2.05	0.56
3:A:494:ASN:HB3	4:B:289:LEU:CD1	2.35	0.56
4:B:393:ILE:HD13	4:B:398:TRP:HB2	1.87	0.56
5:L:89:GLN:HB2	5:L:98:PHE:CD1	2.40	0.56
6:H:6:GLU:HG2	6:H:95:TYR:O	2.04	0.56
3:A:463:ARG:C	3:A:464:GLN:NE2	2.63	0.56
4:B:295:LEU:HD13	4:B:300:GLU:OE1	2.04	0.56
6:H:34:ILE:CG2	6:H:35:GLY:N	2.67	0.56
3:A:429:LEU:HD13	3:A:533:LEU:HD13	1.87	0.56
3:A:536:VAL:HG21	3:A:542:ILE:HG21	1.86	0.56
4:B:324:ASP:O	4:B:343:GLN:HG2	2.05	0.56
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.39	0.56
6:H:164:TRP:CH2	6:H:205:CYS:HB2	2.40	0.56
3:A:329:ILE:HG13	3:A:391:LEU:CD2	2.36	0.56
4:B:111:VAL:HG23	4:B:111:VAL:O	2.04	0.56
6:H:166:SER:N	6:H:206:ASN:HD21	2.01	0.56
4:B:219:LYS:HB3	4:B:232:TYR:CE2	2.40	0.56
3:A:245:VAL:HG23	3:A:245:VAL:O	2.04	0.56
3:A:466:VAL:HG21	3:A:551:LEU:CG	2.35	0.56
1:T:706:DT:H2'	1:T:707:DC:C6	2.41	0.56
2:P:815:DA:C6	2:P:816:DG:C6	2.93	0.56
3:A:492:GLU:HG2	3:A:530:LYS:HB2	1.88	0.56
4:B:112:GLY:HA3	4:B:151:GLN:NE2	2.18	0.56
3:A:63:ILE:HD12	3:A:64:LYS:H	1.71	0.56
3:A:494:ASN:CB	4:B:289:LEU:HD12	2.34	0.56
4:B:2:ILE:HG21	4:B:46:LYS:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:313:PRO:O	4:B:314:VAL:C	2.48	0.56
5:L:83:ILE:HG21	5:L:106:ILE:HG12	1.87	0.56
3:A:328:GLU:HG2	3:A:330:GLN:HE22	1.70	0.56
4:B:291:GLU:O	4:B:293:ILE:N	2.39	0.56
3:A:102:LYS:HG2	3:A:318:TYR:HD1	1.70	0.55
3:A:441:TYR:O	3:A:548:VAL:HG21	2.06	0.55
3:A:466:VAL:CG2	3:A:551:LEU:HG	2.35	0.55
4:B:223:LYS:HB3	5:L:94:PHE:HE1	1.71	0.55
4:B:317:VAL:CG1	4:B:349:LEU:HD23	2.34	0.55
5:L:146:VAL:CG1	5:L:147:LYS:N	2.69	0.55
3:A:317:VAL:HG13	3:A:349:LEU:HD23	1.88	0.55
4:B:231:GLY:O	4:B:232:TYR:C	2.50	0.55
3:A:435:VAL:CG2	4:B:290:THR:HG21	2.24	0.55
3:A:493:VAL:HG22	3:A:494:ASN:N	2.22	0.55
5:L:150:ILE:N	5:L:153:SER:O	2.31	0.55
5:L:108:ARG:HH11	5:L:108:ARG:HG3	1.72	0.55
1:T:704:DC:O2	1:T:704:DC:H2'	2.05	0.55
3:A:364:ASP:HB3	3:A:423:VAL:HG13	1.89	0.55
4:B:393:ILE:HG12	4:B:394:GLN:N	2.22	0.55
6:H:209:HIS:CD2	6:H:212:SER:OG	2.60	0.55
3:A:268:SER:O	3:A:351:THR:O	2.25	0.55
4:B:106:VAL:HA	4:B:189:VAL:O	2.07	0.55
3:A:247:PRO:HB3	3:A:249:LYS:HE3	1.88	0.55
3:A:279:LEU:CD2	3:A:279:LEU:N	2.70	0.55
3:A:417:VAL:O	3:A:417:VAL:HG13	2.07	0.55
3:A:441:TYR:CE2	3:A:544:GLY:N	2.74	0.55
4:B:281:LYS:O	4:B:284:ARG:HB2	2.07	0.55
5:L:165:ASP:O	5:L:166:GLN:C	2.50	0.54
3:A:111:VAL:HG21	3:A:164:MET:HE1	1.89	0.54
4:B:312:GLU:HB3	4:B:315:HIS:CE1	2.42	0.54
4:B:369:THR:O	4:B:373:GLN:HG3	2.07	0.54
6:H:165:ASN:CB	6:H:169:LEU:HD13	2.33	0.54
3:A:301:LEU:O	3:A:305:GLU:HG3	2.06	0.54
4:B:253:THR:HA	4:B:292:VAL:HA	1.90	0.54
6:H:164:TRP:CZ3	6:H:205:CYS:HB2	2.42	0.54
3:A:278:GLN:HE21	3:A:302:GLU:CA	2.21	0.54
4:B:277:ARG:HG3	4:B:278:GLN:H	1.71	0.54
3:A:338:THR:CG2	3:A:339:TYR:N	2.70	0.54
3:A:61:PHE:CZ	3:A:74:LEU:HD23	2.42	0.54
5:L:61:ARG:HB2	5:L:76:SER:CB	2.33	0.54
4:B:191:SER:HB2	4:B:193:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:302:GLU:OE1	4:B:302:GLU:HA	2.08	0.54
3:A:61:PHE:CE2	3:A:74:LEU:HD23	2.43	0.54
4:B:2:ILE:HD12	4:B:3:SER:H	1.73	0.54
5:L:90:GLN:NE2	5:L:93:LYS:H	2.06	0.54
6:H:69:LEU:HD22	6:H:82:LEU:HD11	1.90	0.54
3:A:69:THR:O	3:A:69:THR:HG22	2.08	0.54
3:A:507:GLN:C	3:A:509:GLN:H	2.16	0.54
3:A:406:TRP:CZ2	4:B:420:PRO:HG3	2.43	0.53
4:B:298:GLU:O	4:B:301:LEU:HB3	2.08	0.53
5:L:149:LYS:HE3	5:L:152:GLY:O	2.08	0.53
6:H:69:LEU:HD23	6:H:84:MET:HE3	1.90	0.53
3:A:456:GLY:O	3:A:548:VAL:CG1	2.56	0.53
3:A:454:LYS:C	3:A:552:VAL:HG13	2.34	0.53
5:L:48:ILE:HG21	5:L:52:SER:HA	1.90	0.53
3:A:233:GLU:HB2	3:A:240:THR:CG2	2.34	0.53
3:A:340:GLN:HB3	3:A:348:ASN:OD1	2.08	0.53
4:B:318:TYR:H	4:B:318:TYR:HD2	1.55	0.53
5:L:4:MET:CE	5:L:90:GLN:HB2	2.30	0.53
5:L:193:THR:HG23	5:L:206:VAL:CG1	2.39	0.53
4:B:195:ILE:HG12	4:B:199:ARG:CD	2.39	0.53
4:B:244:ILE:HD11	4:B:310:LEU:HD22	1.89	0.53
3:A:518:VAL:O	3:A:522:ILE:HG13	2.08	0.53
4:B:65:LYS:HA	4:B:407:GLN:OE1	2.08	0.53
4:B:424:LYS:C	4:B:426:TRP:N	2.66	0.53
5:L:205:ILE:N	5:L:205:ILE:HD12	2.23	0.53
3:A:437:ALA:HB1	3:A:492:GLU:O	2.09	0.53
4:B:214:LEU:HD12	4:B:214:LEU:N	2.24	0.53
5:L:62:PHE:CE1	5:L:75:ILE:HG12	2.44	0.53
3:A:222:GLN:O	3:A:223:LYS:C	2.51	0.52
5:L:138:ASN:HD21	6:H:174:HIS:HE1	1.55	0.52
5:L:170:ASP:C	5:L:170:ASP:OD1	2.51	0.52
2:P:820:DC:H2''	2:P:821:DG:H5'	1.90	0.52
5:L:35:TRP:CZ3	5:L:88:CYS:HB3	2.44	0.52
5:L:90:GLN:NE2	5:L:92:SER:N	2.55	0.52
3:A:302:GLU:O	3:A:303:LEU:C	2.52	0.52
3:A:41:MET:HE1	3:A:73:LYS:HD3	1.91	0.52
3:A:215:THR:C	3:A:217:PRO:HD3	2.34	0.52
3:A:477:THR:O	3:A:480:GLN:N	2.40	0.52
3:A:478:GLU:OE1	3:A:498:ASP:OD2	2.26	0.52
4:B:101:LYS:HG3	4:B:102:LYS:HG3	1.90	0.52
4:B:420:PRO:O	4:B:422:LEU:HG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:356:ARG:NE	4:B:360:ALA:HB3	2.22	0.52
4:B:396:GLU:HG2	4:B:396:GLU:O	2.08	0.52
1:T:712:DC:H2'	1:T:713:DT:C6	2.44	0.52
3:A:457:TYR:OH	3:A:488:ASP:OD2	2.15	0.52
6:H:175:THR:HA	6:H:189:SER:HA	1.91	0.52
3:A:503:LEU:HD22	3:A:535:TRP:HB2	1.92	0.52
3:A:454:LYS:HZ2	3:A:554:ALA:HB3	1.74	0.52
4:B:12:LEU:HD11	4:B:127:TYR:CZ	2.44	0.52
4:B:307:ARG:O	4:B:311:LYS:HG3	2.10	0.52
4:B:330:GLN:NE2	4:B:340:GLN:NE2	2.50	0.52
1:T:722:DG:H2''	1:T:723:DA:H8	1.75	0.52
3:A:254:VAL:HG13	3:A:255:ASN:H	1.75	0.52
3:A:465:LYS:O	3:A:466:VAL:CG2	2.57	0.51
4:B:13:LYS:HG2	4:B:83:ARG:O	2.10	0.51
3:A:166:LYS:O	3:A:169:GLU:HB3	2.09	0.51
3:A:227:PHE:HB2	3:A:234:LEU:HB2	1.91	0.51
3:A:493:VAL:CG2	3:A:494:ASN:N	2.74	0.51
1:T:704:DC:C4'	1:T:705:DA:H5'	2.41	0.51
3:A:60:VAL:O	3:A:60:VAL:HG13	2.09	0.51
3:A:257:ILE:O	3:A:261:VAL:HG12	2.10	0.51
3:A:509:GLN:N	3:A:510:PRO:CD	2.73	0.51
4:B:2:ILE:CG2	4:B:46:LYS:HE2	2.41	0.51
4:B:56:TYR:O	4:B:143:ARG:NH2	2.37	0.51
4:B:163:SER:O	4:B:167:ILE:HG13	2.11	0.51
5:L:86:TYR:O	5:L:101:GLY:HA2	2.10	0.51
5:L:108:ARG:HG2	5:L:109:ALA:N	2.26	0.51
3:A:464:GLN:HE21	3:A:464:GLN:N	2.08	0.51
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.93	0.51
1:T:705:DA:H2''	1:T:706:DT:C5'	2.41	0.51
3:A:325:LEU:HD21	3:A:383:TRP:CD2	2.46	0.51
3:A:331:LYS:HD3	3:A:332:GLN:O	2.11	0.51
3:A:361:HIS:CD2	3:A:505:ILE:HG23	2.45	0.51
3:A:434:ILE:HG22	3:A:494:ASN:ND2	2.26	0.51
4:B:146:TYR:CG	4:B:150:PRO:HB3	2.46	0.51
4:B:321:PRO:O	4:B:385:LYS:NZ	2.43	0.51
5:L:46:LEU:HD23	5:L:55:HIS:ND1	2.26	0.51
5:L:117:ILE:HD12	5:L:194:CYS:HB2	1.93	0.51
5:L:34:ASN:HB2	5:L:89:GLN:HE21	1.74	0.51
1:T:708:DG:OP1	3:A:89:GLU:HG3	2.09	0.51
3:A:194:GLU:O	3:A:195:ILE:C	2.54	0.51
3:A:64:LYS:HE2	3:A:66:LYS:HZ3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:330:GLN:HG2	4:B:338:THR:OG1	2.11	0.51
5:L:149:LYS:HA	5:L:154:GLU:HA	1.92	0.51
3:A:221:HIS:N	3:A:221:HIS:CD2	2.78	0.50
3:A:296:THR:O	3:A:299:ALA:HB3	2.11	0.50
4:B:246:LEU:HD12	4:B:307:ARG:HB3	1.93	0.50
6:H:133:PRO:HD3	6:H:218:LYS:HD2	1.93	0.50
1:T:722:DG:H2''	1:T:723:DA:C8	2.46	0.50
3:A:332:GLN:HB2	3:A:336:GLN:HB2	1.92	0.50
3:A:380:ILE:O	3:A:384:GLY:HA2	2.10	0.50
4:B:65:LYS:NZ	4:B:65:LYS:HB3	2.26	0.50
4:B:296:THR:HG22	4:B:297:GLU:N	2.24	0.50
6:H:62:ASN:ND2	6:H:64:SER:H	2.09	0.50
3:A:35:VAL:HG23	3:A:132:ILE:HD11	1.92	0.50
3:A:41:MET:HE1	3:A:73:LYS:NZ	2.27	0.50
3:A:427:TYR:CE1	3:A:525:LEU:HD23	2.47	0.50
3:A:533:LEU:N	3:A:533:LEU:CD1	2.73	0.50
4:B:195:ILE:CG2	4:B:196:GLY:N	2.74	0.50
1:T:704:DC:C5'	1:T:705:DA:H5'	2.42	0.50
3:A:257:ILE:CG2	3:A:283:LEU:HD21	2.41	0.50
5:L:34:ASN:HD22	5:L:89:GLN:NE2	1.92	0.50
6:H:172:GLY:O	6:H:191:VAL:HA	2.11	0.50
6:H:212:SER:O	6:H:214:THR:HG23	2.12	0.50
1:T:705:DA:H2''	1:T:706:DT:H5'	1.93	0.50
3:A:457:TYR:CE2	3:A:465:LYS:HB3	2.47	0.50
5:L:120:PRO:O	5:L:121:SER:O	2.30	0.50
6:H:6:GLU:OE2	6:H:114:GLY:HA3	2.11	0.50
6:H:155:TYR:CE1	6:H:160:VAL:HG13	2.46	0.50
3:A:49:LYS:HB2	3:A:49:LYS:HZ3	1.76	0.50
3:A:474:ASN:OD1	3:A:474:ASN:N	2.43	0.50
4:B:160:PHE:HE2	4:B:164:MET:HE2	1.77	0.50
4:B:353:LYS:O	4:B:353:LYS:HG3	2.11	0.50
5:L:27:GLN:O	5:L:28:ASP:C	2.55	0.50
5:L:90:GLN:NE2	5:L:92:SER:H	1.93	0.50
3:A:416:PHE:CZ	3:A:418:ASN:HA	2.46	0.50
4:B:100:LEU:HD13	4:B:381:VAL:HG13	1.94	0.50
5:L:135:PHE:HB3	5:L:137:ASN:HD21	1.77	0.50
3:A:466:VAL:O	3:A:466:VAL:CG1	2.55	0.49
3:A:472:THR:HB	3:A:476:LYS:HB2	1.93	0.49
4:B:87:PHE:HZ	4:B:159:ILE:HG13	1.77	0.49
5:L:138:ASN:ND2	5:L:138:ASN:N	2.59	0.49
5:L:161:ASN:ND2	5:L:175:MET:HE3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:806:DC:C2	2:P:807:DC:C5	3.00	0.49
3:A:247:PRO:HG2	3:A:259:LYS:HE2	1.93	0.49
5:L:31:SER:HA	5:L:51:THR:OG1	2.12	0.49
3:A:420:PRO:HA	3:A:421:PRO:C	2.36	0.49
4:B:219:LYS:HB3	4:B:232:TYR:HE2	1.78	0.49
5:L:205:ILE:HD12	5:L:205:ILE:H	1.78	0.49
3:A:350:LYS:HE2	3:A:378:GLU:OE1	2.11	0.49
5:L:190:ASN:O	5:L:210:ASN:HA	2.13	0.49
3:A:420:PRO:HB3	3:A:421:PRO:HA	1.94	0.49
3:A:517:LEU:C	3:A:517:LEU:HD13	2.37	0.49
4:B:263:LYS:HA	4:B:423:VAL:HG11	1.94	0.49
3:A:350:LYS:CE	3:A:378:GLU:OE1	2.60	0.49
4:B:376:THR:O	4:B:380:ILE:HG13	2.12	0.49
5:L:58:VAL:HG13	5:L:59:PRO:HD2	1.94	0.49
3:A:136:ASN:HB2	3:A:138:GLU:HG3	1.94	0.49
3:A:552:VAL:C	3:A:554:ALA:H	2.20	0.49
4:B:393:ILE:CG1	4:B:394:GLN:N	2.75	0.49
6:H:152:VAL:HB	6:H:187:LEU:HD13	1.95	0.49
6:H:165:ASN:HD22	6:H:169:LEU:CD1	2.25	0.49
6:H:169:LEU:N	6:H:169:LEU:HD12	2.28	0.49
3:A:76:ASP:OD1	3:A:78:ARG:HG3	2.13	0.49
3:A:171:PHE:CE2	3:A:205:LEU:HD13	2.48	0.49
3:A:410:TRP:HB3	4:B:365:VAL:HG23	1.95	0.49
4:B:113:ASP:O	4:B:114:ALA:C	2.54	0.49
4:B:317:VAL:HG11	4:B:348:ASN:O	2.13	0.49
5:L:45:LYS:HG2	5:L:46:LEU:N	2.26	0.49
1:T:708:DG:H2'	1:T:709:DG:C8	2.48	0.49
3:A:331:LYS:HB3	3:A:421:PRO:HG2	1.95	0.49
3:A:463:ARG:CG	3:A:464:GLN:N	2.76	0.49
4:B:210:LEU:C	4:B:212:TRP:N	2.68	0.49
5:L:190:ASN:CG	5:L:210:ASN:HD22	2.20	0.49
6:H:34:ILE:HG22	6:H:35:GLY:N	2.27	0.49
6:H:53:ILE:HA	6:H:59:ASN:ND2	2.28	0.49
3:A:447:ASN:HB3	3:A:450:THR:OG1	2.13	0.49
4:B:104:LYS:HB3	4:B:104:LYS:HZ3	1.77	0.49
6:H:107:ASP:HB3	9:H:1725:GLC:O3	2.13	0.49
3:A:24:TRP:HZ3	3:A:61:PHE:CB	2.22	0.48
4:B:223:LYS:NZ	6:H:56:ASP:OD2	2.46	0.48
4:B:304:ALA:HA	4:B:307:ARG:HE	1.78	0.48
3:A:441:TYR:CD2	3:A:544:GLY:HA3	2.47	0.48
5:L:14:SER:O	5:L:15:LEU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:12:VAL:HG21	6:H:18:PHE:HB3	1.95	0.48
3:A:27:THR:HG23	3:A:30:LYS:HD2	1.95	0.48
3:A:541:GLY:HA2	3:A:546:GLU:HG3	1.96	0.48
4:B:333:GLY:O	4:B:334:GLN:HB2	2.13	0.48
5:L:15:LEU:HD12	5:L:15:LEU:N	2.13	0.48
5:L:49:TYR:O	5:L:50:TYR:HB3	2.13	0.48
4:B:357:MET:SD	4:B:370:GLU:OE1	2.71	0.48
3:A:339:TYR:CD2	3:A:375:ILE:HD11	2.49	0.48
4:B:278:GLN:HB3	4:B:279:LEU:HD12	1.95	0.48
5:L:45:LYS:HG2	5:L:46:LEU:H	1.78	0.48
5:L:198:HIS:C	5:L:200:THR:H	2.22	0.48
4:B:285:GLY:H	4:B:287:LYS:HZ2	1.61	0.48
5:L:151:ASP:CA	5:L:191:SER:HB3	2.43	0.48
5:L:175:MET:HE3	5:L:177:SER:HB2	1.96	0.48
3:A:40:GLU:OE1	3:A:40:GLU:HA	2.14	0.48
3:A:96:HIS:CG	3:A:97:PRO:HD2	2.48	0.48
3:A:181:TYR:CD1	4:B:138:GLU:HA	2.48	0.48
5:L:138:ASN:HD22	5:L:138:ASN:N	2.12	0.48
6:H:209:HIS:CE1	6:H:211:ALA:HB3	2.49	0.48
2:P:816:DG:H2'	2:P:817:DC:H6	1.77	0.48
3:A:109:LEU:HD23	3:A:220:LYS:HB2	1.96	0.48
3:A:363:ASN:OD1	3:A:363:ASN:C	2.57	0.48
4:B:104:LYS:O	4:B:235:HIS:HD2	1.96	0.48
4:B:210:LEU:O	4:B:212:TRP:N	2.39	0.48
5:L:36:TYR:HE2	5:L:89:GLN:HB3	1.78	0.48
2:P:807:DC:C4'	3:A:448:ARG:HD2	2.36	0.47
3:A:23:GLN:HE22	3:A:60:VAL:N	2.05	0.47
3:A:97:PRO:HA	3:A:100:LEU:HD12	1.96	0.47
3:A:7:THR:CG2	3:A:119:PRO:HB2	2.43	0.47
3:A:132:ILE:HG23	3:A:142:ILE:HB	1.95	0.47
3:A:235:HIS:HB2	3:A:238:LYS:O	2.13	0.47
4:B:171:PHE:CE1	4:B:205:LEU:HA	2.49	0.47
4:B:195:ILE:HG23	4:B:196:GLY:N	2.29	0.47
4:B:420:PRO:HB3	4:B:421:PRO:HD2	1.95	0.47
5:L:61:ARG:HG2	5:L:61:ARG:HH11	1.79	0.47
3:A:343:GLN:HE21	3:A:349:LEU:HD21	1.80	0.47
3:A:429:LEU:HD11	3:A:506:ILE:HG22	1.94	0.47
3:A:516:GLU:O	3:A:519:ASN:N	2.47	0.47
3:A:543:GLY:C	3:A:545:ASN:H	2.23	0.47
4:B:263:LYS:CA	4:B:423:VAL:HG11	2.45	0.47
4:B:363:ASN:HD21	4:B:365:VAL:HB	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:418:ASN:C	4:B:418:ASN:HD22	2.20	0.47
6:H:40:ARG:HB2	6:H:50:LEU:HD11	1.95	0.47
1:T:719:DA:H2''	1:T:720:DG:O5'	2.14	0.47
3:A:357:MET:HG3	3:A:367:GLN:HE22	1.80	0.47
4:B:101:LYS:O	4:B:236:PRO:CB	2.61	0.47
5:L:23:CYS:HB2	5:L:35:TRP:CH2	2.49	0.47
3:A:497:THR:HG22	3:A:498:ASP:H	1.79	0.47
4:B:187:LEU:HD12	4:B:187:LEU:HA	1.76	0.47
5:L:199:LYS:O	5:L:199:LYS:CG	2.61	0.47
6:H:134:LEU:HD12	6:H:149:GLY:HA3	1.95	0.47
4:B:151:GLN:HB3	4:B:185:ASP:OD2	2.15	0.47
4:B:326:ILE:N	4:B:326:ILE:HD12	2.30	0.47
5:L:175:MET:CE	5:L:177:SER:HB2	2.45	0.47
3:A:319:TYR:HA	3:A:343:GLN:HE22	1.80	0.47
3:A:486:LEU:CD1	3:A:521:ILE:HG23	2.45	0.47
4:B:79:GLU:O	4:B:83:ARG:HG2	2.15	0.47
4:B:206:ARG:NH1	4:B:216:THR:O	2.48	0.47
4:B:330:GLN:HE22	4:B:340:GLN:CD	2.21	0.47
6:H:31:THR:HB	6:H:34:ILE:HD12	1.96	0.47
2:P:815:DA:H2'	2:P:816:DG:C8	2.50	0.47
3:A:5:ILE:HD11	3:A:167:ILE:CD1	2.32	0.47
3:A:547:GLN:HE21	3:A:547:GLN:CA	2.28	0.47
4:B:175:ASN:C	4:B:177:ASP:N	2.73	0.47
4:B:330:GLN:CG	4:B:338:THR:OG1	2.63	0.47
5:L:128:GLY:C	5:L:183:LYS:HB2	2.40	0.46
2:P:822:2DA:H3'1	3:A:185:ASP:OD1	2.14	0.46
3:A:328:GLU:HG3	3:A:390:LYS:HB2	1.96	0.46
4:B:225:PRO:HB2	5:L:32:TYR:CE1	2.51	0.46
3:A:13:LYS:HD2	3:A:16:MET:CE	2.43	0.46
3:A:129:ALA:HA	3:A:144:TYR:O	2.16	0.46
3:A:473:THR:OG1	3:A:476:LYS:HG2	2.14	0.46
4:B:175:ASN:HD21	4:B:201:LYS:HZ1	1.61	0.46
4:B:277:ARG:HG3	4:B:278:GLN:N	2.31	0.46
4:B:394:GLN:O	4:B:395:LYS:C	2.58	0.46
3:A:278:GLN:H	3:A:278:GLN:HG2	1.34	0.46
3:A:339:TYR:CD2	3:A:375:ILE:CD1	2.99	0.46
5:L:11:LEU:HD21	5:L:19:VAL:CG1	2.45	0.46
6:H:150:CYS:HB2	6:H:164:TRP:CZ2	2.50	0.46
3:A:31:ILE:O	3:A:35:VAL:HG23	2.16	0.46
3:A:473:THR:H	3:A:476:LYS:HB2	1.80	0.46
4:B:299:ALA:O	4:B:300:GLU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:201:SER:C	5:L:203:SER:H	2.23	0.46
1:T:705:DA:H2''	1:T:706:DT:O5'	2.15	0.46
3:A:490:GLY:C	3:A:492:GLU:H	2.24	0.46
4:B:154:LYS:HA	4:B:184:MET:HE3	1.97	0.46
4:B:183:TYR:CD2	4:B:380:ILE:HD13	2.50	0.46
4:B:285:GLY:O	4:B:287:LYS:N	2.49	0.46
4:B:330:GLN:NE2	4:B:340:GLN:CD	2.74	0.46
4:B:424:LYS:O	4:B:425:LEU:C	2.58	0.46
5:L:2:ILE:HG23	5:L:27:GLN:HG3	1.98	0.46
6:H:14:PRO:O	6:H:15:SER:HB2	2.15	0.46
6:H:40:ARG:HD3	6:H:50:LEU:HD11	1.97	0.46
3:A:461:LYS:O	3:A:463:ARG:N	2.48	0.46
4:B:260:LEU:HG	4:B:260:LEU:O	2.16	0.46
4:B:363:ASN:C	4:B:363:ASN:ND2	2.67	0.46
5:L:120:PRO:O	5:L:121:SER:C	2.59	0.46
5:L:136:LEU:HD21	5:L:146:VAL:HG22	1.97	0.46
3:A:269:GLN:HA	3:A:351:THR:O	2.14	0.46
5:L:61:ARG:HH21	5:L:82:ASP:CG	2.24	0.46
6:H:62:ASN:HD22	6:H:63:PRO:CD	2.28	0.46
6:H:142:THR:HG22	6:H:143:ASN:N	2.31	0.46
2:P:804:DG:H2'	2:P:805:DT:H71	1.96	0.46
3:A:12:LEU:HD11	3:A:127:TYR:CZ	2.51	0.46
3:A:257:ILE:HG22	3:A:283:LEU:HD21	1.97	0.46
3:A:412:PRO:O	3:A:413:GLU:C	2.59	0.46
4:B:75:VAL:HG11	4:B:77:PHE:CE2	2.51	0.46
4:B:146:TYR:CD2	4:B:150:PRO:HB3	2.51	0.46
5:L:78:LEU:HD21	5:L:104:LEU:HD21	1.98	0.46
5:L:190:ASN:HD22	5:L:211:ARG:HG2	1.79	0.46
3:A:442:VAL:HB	3:A:481:ALA:HB1	1.96	0.45
3:A:529:GLU:O	3:A:530:LYS:CG	2.64	0.45
4:B:118:VAL:O	4:B:148:VAL:HA	2.15	0.45
4:B:199:ARG:HH12	4:B:229:TRP:HZ3	1.63	0.45
5:L:98:PHE:CZ	6:H:110:MET:HE1	2.51	0.45
5:L:206:VAL:HG12	5:L:207:LYS:N	2.31	0.45
6:H:42:PRO:HA	6:H:93:ALA:HB2	1.96	0.45
3:A:50:ILE:HG23	3:A:145:GLN:HB3	1.98	0.45
3:A:134:SER:C	3:A:136:ASN:N	2.74	0.45
3:A:297:GLU:HA	3:A:300:GLU:CB	2.42	0.45
3:A:305:GLU:O	3:A:308:GLU:HB2	2.16	0.45
4:B:368:LEU:O	4:B:372:VAL:HG23	2.16	0.45
5:L:51:THR:HG23	5:L:71:TYR:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:112:GLY:O	3:A:113:ASP:HB2	2.15	0.45
3:A:139:THR:HG23	3:A:140:PRO:CD	2.46	0.45
3:A:257:ILE:HD13	3:A:282:LEU:HB2	1.97	0.45
3:A:516:GLU:O	3:A:517:LEU:C	2.59	0.45
3:A:545:ASN:O	3:A:546:GLU:C	2.58	0.45
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.52	0.45
4:B:214:LEU:N	4:B:214:LEU:CD1	2.78	0.45
4:B:276:VAL:HG12	4:B:276:VAL:O	2.16	0.45
5:L:125:LEU:HD23	5:L:129:GLY:O	2.16	0.45
5:L:160:LEU:HD11	6:H:181:GLN:CD	2.42	0.45
6:H:54:TRP:H	6:H:59:ASN:HD22	1.64	0.45
3:A:536:VAL:HG11	3:A:542:ILE:HB	1.97	0.45
5:L:6:GLN:HA	5:L:22:SER:O	2.17	0.45
6:H:42:PRO:HA	6:H:93:ALA:CB	2.47	0.45
4:B:39:THR:O	4:B:42:GLU:HB3	2.16	0.45
5:L:115:VAL:HG12	5:L:207:LYS:HG3	1.99	0.45
1:T:712:DC:OP1	3:A:353:LYS:NZ	2.49	0.45
4:B:135:ILE:O	4:B:135:ILE:CD1	2.57	0.45
4:B:160:PHE:O	4:B:160:PHE:CD2	2.70	0.45
3:A:134:SER:O	3:A:136:ASN:N	2.50	0.45
4:B:46:LYS:HD2	4:B:148:VAL:CG2	2.44	0.45
4:B:264:LEU:O	4:B:274:ILE:HG21	2.17	0.45
3:A:96:HIS:ND1	3:A:97:PRO:HD2	2.31	0.45
3:A:264:LEU:O	3:A:267:ALA:HB3	2.17	0.45
3:A:478:GLU:HG2	3:A:499:SER:HB3	1.98	0.45
3:A:66:LYS:HA	3:A:66:LYS:HD3	1.77	0.45
3:A:435:VAL:HG22	4:B:290:THR:CB	2.46	0.45
5:L:11:LEU:HD23	5:L:104:LEU:HD13	1.99	0.45
6:H:129:PRO:HB2	6:H:152:VAL:CG1	2.47	0.45
3:A:547:GLN:HE21	3:A:547:GLN:H	1.59	0.44
4:B:170:PRO:HB2	4:B:208:HIS:CE1	2.52	0.44
4:B:258:GLN:HG2	4:B:283:LEU:CD1	2.48	0.44
4:B:282:LEU:N	4:B:282:LEU:HD23	2.33	0.44
5:L:63:SER:O	5:L:73:LEU:HD12	2.16	0.44
6:H:174:HIS:O	6:H:189:SER:HA	2.17	0.44
3:A:482:ILE:O	3:A:486:LEU:HG	2.17	0.44
4:B:27:THR:OG1	4:B:30:LYS:HG3	2.16	0.44
4:B:193:LEU:HD12	4:B:198:HIS:HA	1.99	0.44
3:A:23:GLN:HG2	3:A:133:PRO:HD3	1.99	0.44
3:A:108:VAL:O	3:A:109:LEU:HD23	2.18	0.44
3:A:406:TRP:NE1	4:B:418:ASN:HD21	2.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:129:PRO:HB2	6:H:152:VAL:HG13	1.97	0.44
3:A:408:ALA:HB1	4:B:364:ASP:HB3	1.98	0.44
3:A:452:LEU:HD23	3:A:470:THR:HG22	1.99	0.44
4:B:132:ILE:HA	4:B:133:PRO:HD3	1.79	0.44
4:B:212:TRP:O	4:B:212:TRP:HD1	1.99	0.44
5:L:4:MET:HE1	5:L:29:ILE:HD13	1.99	0.44
3:A:419:THR:O	3:A:419:THR:HG22	2.18	0.44
4:B:87:PHE:CE1	4:B:92:LEU:HD12	2.53	0.44
5:L:91:TYR:OH	6:H:106:THR:O	2.32	0.44
3:A:389:PHE:O	3:A:414:TRP:HA	2.17	0.44
5:L:151:ASP:OD2	5:L:189:HIS:ND1	2.51	0.44
6:H:128:PRO:HA	6:H:209:HIS:CD2	2.50	0.44
3:A:254:VAL:O	3:A:257:ILE:HB	2.18	0.44
3:A:337:TRP:CZ2	3:A:367:GLN:HB2	2.53	0.44
3:A:393:ILE:HG23	3:A:393:ILE:O	2.17	0.44
3:A:411:ILE:HG22	3:A:412:PRO:O	2.16	0.44
3:A:507:GLN:C	3:A:509:GLN:N	2.74	0.44
4:B:3:SER:HA	4:B:4:PRO:HD3	1.88	0.44
4:B:221:HIS:HA	4:B:229:TRP:CD1	2.52	0.44
4:B:325:LEU:HD12	4:B:343:GLN:HG2	2.00	0.44
5:L:139:PHE:CD1	5:L:139:PHE:C	2.96	0.44
6:H:173:VAL:HA	6:H:190:SER:O	2.18	0.44
2:P:816:DG:H2'	2:P:817:DC:C6	2.52	0.44
3:A:261:VAL:HG23	3:A:276:VAL:CG1	2.47	0.44
3:A:454:LYS:O	3:A:552:VAL:CG1	2.66	0.44
3:A:541:GLY:HA2	3:A:546:GLU:CG	2.48	0.44
4:B:100:LEU:HD22	4:B:100:LEU:O	2.18	0.44
4:B:120:LEU:O	4:B:121:ASP:C	2.61	0.44
4:B:395:LYS:HA	4:B:416:PHE:CE1	2.53	0.44
3:A:167:ILE:O	3:A:170:PRO:HD2	2.18	0.43
4:B:29:GLU:HG2	4:B:71:TRP:CH2	2.53	0.43
1:T:711:DG:H2'	1:T:712:DC:H6	1.83	0.43
3:A:452:LEU:HB3	3:A:470:THR:HG22	2.00	0.43
4:B:68:SER:O	4:B:69:THR:HB	2.18	0.43
4:B:96:HIS:HA	4:B:97:PRO:HD3	1.86	0.43
4:B:175:ASN:OD1	4:B:201:LYS:HE3	2.18	0.43
4:B:414:TRP:CD1	4:B:414:TRP:C	2.95	0.43
3:A:281:LYS:NZ	3:A:284:ARG:CB	2.81	0.43
3:A:555:GLY:O	3:A:556:ILE:CG1	2.61	0.43
4:B:97:PRO:HG2	4:B:181:TYR:HB2	1.99	0.43
4:B:103:LYS:HA	4:B:103:LYS:CE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:9:PRO:O	6:H:11:ILE:N	2.47	0.43
5:L:21:ILE:HD13	5:L:102:THR:HB	2.00	0.43
5:L:198:HIS:O	5:L:200:THR:N	2.47	0.43
3:A:118:VAL:HA	3:A:119:PRO:HD3	1.79	0.43
4:B:235:HIS:C	4:B:237:ASP:H	2.26	0.43
4:B:350:LYS:HE2	4:B:378:GLU:OE1	2.18	0.43
3:A:49:LYS:HB2	3:A:49:LYS:HZ2	1.83	0.43
3:A:162:SER:OG	4:B:52:PRO:HD3	2.18	0.43
3:A:206:ARG:NH2	3:A:216:THR:O	2.52	0.43
3:A:278:GLN:HE21	3:A:302:GLU:CB	2.32	0.43
3:A:458:VAL:HG11	3:A:547:GLN:HG2	2.00	0.43
4:B:154:LYS:HG2	4:B:184:MET:CE	2.48	0.43
4:B:278:GLN:HG3	4:B:299:ALA:HA	1.99	0.43
3:A:199:ARG:NH2	3:A:220:LYS:CE	2.76	0.43
3:A:338:THR:HG22	3:A:340:GLN:NE2	2.34	0.43
5:L:147:LYS:HZ2	5:L:149:LYS:HD2	1.77	0.43
6:H:39:ILE:HG22	6:H:40:ARG:N	2.33	0.43
6:H:84:MET:HG2	6:H:87:VAL:CG1	2.40	0.43
3:A:455:ALA:HB3	3:A:469:LEU:HD11	2.01	0.43
3:A:506:ILE:O	3:A:510:PRO:HD2	2.19	0.43
4:B:116:PHE:C	4:B:148:VAL:HG11	2.43	0.43
5:L:144:ILE:HG13	5:L:198:HIS:ND1	2.34	0.43
5:L:201:SER:C	5:L:203:SER:N	2.74	0.43
6:H:60:ARG:HD3	6:H:60:ARG:HA	1.73	0.43
5:L:89:GLN:HB2	5:L:98:PHE:CE1	2.54	0.43
5:L:118:PHE:HA	5:L:119:PRO:HD3	1.83	0.43
1:T:711:DG:H2'	1:T:712:DC:C6	2.54	0.43
3:A:5:ILE:CD1	3:A:167:ILE:HD11	2.32	0.43
3:A:41:MET:HE1	3:A:73:LYS:CD	2.48	0.43
3:A:459:THR:HG23	3:A:463:ARG:CB	2.30	0.43
3:A:465:LYS:HD2	3:A:467:VAL:HG13	2.00	0.43
4:B:306:ASN:O	4:B:309:ILE:N	2.45	0.43
3:A:47:ILE:HD12	3:A:144:TYR:CD1	2.54	0.42
3:A:257:ILE:HD13	3:A:282:LEU:CB	2.49	0.42
3:A:427:TYR:CZ	3:A:525:LEU:HD23	2.54	0.42
4:B:2:ILE:HD12	4:B:2:ILE:N	2.32	0.42
4:B:154:LYS:HG2	4:B:184:MET:HE3	2.01	0.42
1:T:712:DC:H42	2:P:815:DA:N6	2.17	0.42
3:A:11:LYS:H	3:A:85:GLN:HG2	1.83	0.42
4:B:43:LYS:C	4:B:45:GLY:H	2.25	0.42
4:B:239:TRP:CZ2	4:B:378:GLU:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:279:LEU:H	4:B:279:LEU:CD1	2.32	0.42
5:L:1:ASP:N	5:L:95:PRO:HG2	2.34	0.42
5:L:61:ARG:CZ	5:L:79:GLU:HG3	2.49	0.42
5:L:150:ILE:HA	5:L:191:SER:O	2.18	0.42
5:L:190:ASN:CG	5:L:210:ASN:ND2	2.77	0.42
4:B:171:PHE:C	4:B:171:PHE:CD2	2.97	0.42
3:A:109:LEU:CD2	3:A:220:LYS:HB2	2.48	0.42
3:A:181:TYR:HB2	3:A:188:TYR:HB3	2.00	0.42
3:A:245:VAL:O	3:A:245:VAL:CG2	2.67	0.42
3:A:438:GLU:HG2	3:A:461:LYS:CD	2.49	0.42
4:B:210:LEU:HD12	4:B:210:LEU:HA	1.62	0.42
4:B:423:VAL:C	4:B:425:LEU:H	2.28	0.42
5:L:135:PHE:HB3	5:L:137:ASN:ND2	2.34	0.42
3:A:460:ASN:HA	4:B:286:THR:OG1	2.19	0.42
5:L:182:THR:HG22	5:L:183:LYS:N	2.33	0.42
6:H:2:ILE:HG21	6:H:112:HIS:HD2	1.83	0.42
4:B:260:LEU:CD2	4:B:303:LEU:HD13	2.35	0.42
5:L:54:LEU:HD22	5:L:54:LEU:HA	1.80	0.42
5:L:149:LYS:HD3	5:L:195:GLU:OE2	2.19	0.42
6:H:39:ILE:HG13	6:H:113:TRP:CH2	2.55	0.42
6:H:153:LYS:NZ	10:H:1726:HOH:O	2.45	0.42
6:H:199:PRO:C	6:H:201:GLU:N	2.76	0.42
3:A:201:LYS:HA	3:A:201:LYS:HD2	1.84	0.42
3:A:409:THR:HG23	10:A:563:HOH:O	2.19	0.42
4:B:206:ARG:NH1	4:B:217:PRO:O	2.53	0.42
4:B:319:TYR:CZ	4:B:383:TRP:HB3	2.54	0.42
5:L:124:GLN:HE22	5:L:131:SER:CB	2.32	0.42
3:A:10:VAL:HG11	3:A:153:TRP:HZ2	1.85	0.42
3:A:265:ASN:C	3:A:268:SER:HG	2.25	0.42
3:A:418:ASN:O	3:A:419:THR:OG1	2.31	0.42
3:A:547:GLN:H	3:A:547:GLN:NE2	2.18	0.42
4:B:50:ILE:CG2	4:B:145:GLN:HG2	2.47	0.42
4:B:115:TYR:C	4:B:117:SER:H	2.28	0.42
2:P:808:DC:H4'	3:A:475:GLN:OE1	2.18	0.42
3:A:253:THR:O	3:A:254:VAL:C	2.61	0.42
3:A:523:GLU:OE1	3:A:523:GLU:HA	2.20	0.42
4:B:156:SER:N	4:B:157:PRO:HD2	2.34	0.42
5:L:118:PHE:HZ	6:H:147:THR:O	2.03	0.42
3:A:194:GLU:C	3:A:196:GLY:N	2.78	0.42
3:A:457:TYR:HA	3:A:548:VAL:HG11	2.02	0.42
3:A:458:VAL:HG11	3:A:547:GLN:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:ILE:H	3:A:542:ILE:HD12	1.85	0.42
4:B:167:ILE:O	4:B:208:HIS:NE2	2.45	0.42
4:B:266:TRP:HH2	4:B:422:LEU:CD2	2.26	0.42
3:A:344:GLU:HA	3:A:345:PRO:HD2	1.79	0.41
3:A:494:ASN:OD1	4:B:289:LEU:HD12	2.20	0.41
4:B:7:THR:HG22	4:B:119:PRO:HG2	2.02	0.41
4:B:212:TRP:O	4:B:212:TRP:CD1	2.72	0.41
4:B:305:GLU:O	4:B:306:ASN:C	2.62	0.41
5:L:90:GLN:HE22	5:L:93:LYS:H	1.66	0.41
6:H:174:HIS:O	6:H:190:SER:N	2.50	0.41
2:P:810:DG:OP1	3:A:361:HIS:NE2	2.48	0.41
3:A:28:GLU:CD	3:A:135:ILE:HD11	2.46	0.41
3:A:139:THR:O	3:A:140:PRO:C	2.62	0.41
3:A:279:LEU:H	3:A:279:LEU:HD22	1.84	0.41
4:B:263:LYS:HB2	4:B:423:VAL:CG1	2.50	0.41
3:A:111:VAL:CG1	3:A:214:LEU:HD12	2.38	0.41
3:A:188:TYR:CD1	3:A:188:TYR:C	2.98	0.41
3:A:317:VAL:HG12	3:A:348:ASN:O	2.20	0.41
3:A:325:LEU:HB3	3:A:387:PRO:HB3	2.01	0.41
3:A:441:TYR:O	3:A:548:VAL:HG11	2.20	0.41
4:B:195:ILE:HG12	4:B:199:ARG:HE	1.83	0.41
3:A:400:THR:C	3:A:403:THR:HG22	2.46	0.41
3:A:526:ILE:O	3:A:526:ILE:HG12	2.19	0.41
4:B:27:THR:O	4:B:28:GLU:C	2.64	0.41
5:L:146:VAL:CG1	5:L:147:LYS:H	2.34	0.41
6:H:86:THR:O	6:H:86:THR:HG22	2.20	0.41
4:B:47:ILE:HA	4:B:145:GLN:O	2.21	0.41
6:H:54:TRP:H	6:H:59:ASN:ND2	2.19	0.41
3:A:295:LEU:O	3:A:296:THR:C	2.63	0.41
3:A:491:LEU:O	3:A:529:GLU:HB2	2.19	0.41
5:L:138:ASN:HA	5:L:173:TYR:O	2.20	0.41
3:A:416:PHE:HZ	3:A:422:LEU:HD11	1.85	0.41
3:A:511:ASP:OD2	3:A:512:LYS:HE3	2.20	0.41
3:A:542:ILE:HD12	3:A:542:ILE:N	2.36	0.41
3:A:548:VAL:O	3:A:552:VAL:HG23	2.21	0.41
3:A:472:THR:O	3:A:473:THR:HG23	2.20	0.41
3:A:495:ILE:O	3:A:496:VAL:HG23	2.21	0.41
5:L:151:ASP:C	5:L:153:SER:H	2.27	0.41
5:L:188:ARG:O	5:L:189:HIS:CG	2.74	0.41
6:H:169:LEU:CD1	6:H:169:LEU:N	2.83	0.41
3:A:113:ASP:O	3:A:114:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:458:VAL:HG23	3:A:548:VAL:HG13	2.03	0.41
3:A:465:LYS:C	3:A:466:VAL:HG23	2.46	0.41
4:B:104:LYS:O	4:B:235:HIS:CD2	2.74	0.41
4:B:241:VAL:HA	4:B:351:THR:O	2.20	0.41
5:L:31:SER:CA	5:L:51:THR:OG1	2.69	0.41
5:L:48:ILE:HG23	5:L:53:SER:O	2.20	0.41
5:L:135:PHE:C	5:L:136:LEU:HD12	2.45	0.41
6:H:28:SER:C	6:H:30:SER:H	2.29	0.41
6:H:40:ARG:HD2	6:H:95:TYR:CZ	2.56	0.41
6:H:105:VAL:HG12	6:H:105:VAL:O	2.20	0.41
6:H:204:THR:HG23	6:H:218:LYS:O	2.21	0.41
3:A:8:VAL:HA	3:A:9:PRO:HD3	1.89	0.41
3:A:10:VAL:HG11	3:A:153:TRP:CZ2	2.56	0.41
3:A:134:SER:O	3:A:135:ILE:C	2.64	0.41
4:B:8:VAL:HA	4:B:9:PRO:HD3	1.69	0.41
4:B:34:LEU:HD13	4:B:62:ALA:HB2	2.02	0.41
4:B:125:ARG:HD3	4:B:146:TYR:O	2.21	0.41
4:B:146:TYR:CE2	4:B:150:PRO:HA	2.56	0.41
4:B:178:ILE:CD1	4:B:201:LYS:HG2	2.45	0.41
4:B:242:GLN:CD	4:B:353:LYS:HD2	2.46	0.41
4:B:282:LEU:HD21	4:B:299:ALA:HB2	2.02	0.41
5:L:91:TYR:CE1	6:H:108:SER:HB3	2.56	0.41
2:P:804:DG:H2''	2:P:805:DT:O5'	2.21	0.40
4:B:34:LEU:HD12	4:B:34:LEU:HA	1.70	0.40
4:B:88:TRP:CD1	4:B:154:LYS:HB2	2.56	0.40
4:B:129:ALA:HA	4:B:144:TYR:O	2.21	0.40
4:B:175:ASN:HD21	4:B:201:LYS:HZ2	1.64	0.40
4:B:414:TRP:CD1	4:B:414:TRP:O	2.74	0.40
5:L:170:ASP:O	5:L:172:THR:HG23	2.21	0.40
3:A:434:ILE:CG2	3:A:494:ASN:ND2	2.82	0.40
6:H:216:VAL:HG12	6:H:217:ASP:N	2.36	0.40
3:A:68:SER:O	3:A:69:THR:HB	2.21	0.40
3:A:333:GLY:O	3:A:334:GLN:C	2.64	0.40
3:A:470:THR:O	3:A:471:ASN:HB2	2.21	0.40
3:A:484:LEU:O	3:A:486:LEU:N	2.55	0.40
4:B:169:GLU:N	4:B:170:PRO:CD	2.84	0.40
5:L:55:HIS:CD2	5:L:56:SER:H	2.39	0.40
4:B:46:LYS:HD3	4:B:46:LYS:HA	1.63	0.40
4:B:125:ARG:NH1	4:B:147:ASN:OD1	2.54	0.40
6:H:91:ASP:HB2	6:H:121:VAL:HG21	2.02	0.40
3:A:80:LEU:O	3:A:84:THR:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:281:LYS:HD3	3:A:284:ARG:CB	2.52	0.40
3:A:297:GLU:CA	3:A:300:GLU:HB2	2.47	0.40
4:B:257:ILE:HG12	4:B:257:ILE:H	1.69	0.40
4:B:301:LEU:HG	4:B:302:GLU:OE1	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2:ILE:O	4:B:2:ILE:O[6_565]	1.96	0.24
4:B:3:SER:OG	4:B:3:SER:OG[6_565]	2.02	0.18

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	
3	A	556/558 (100%)	456 (82%)	69 (12%)	31 (6%)	1	4
4	B	427/429 (100%)	361 (84%)	52 (12%)	14 (3%)	3	11
5	L	209/211 (99%)	184 (88%)	18 (9%)	7 (3%)	3	11
6	H	223/225 (99%)	198 (89%)	22 (10%)	3 (1%)	9	31
All	All	1415/1423 (99%)	1199 (85%)	161 (11%)	55 (4%)	2	8

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	273	GLY
3	A	278	GLN
3	A	286	THR
3	A	345	PRO
3	A	466	VAL

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Mol	Chain	Res	Type
3	A	474	ASN
4	B	247	PRO
4	B	286	THR
4	B	292	VAL
4	B	355	ALA
5	L	76	SER
5	L	121	SER
3	A	195	ILE
3	A	462	GLY
3	A	543	GLY
3	A	547	GLN
3	A	556	ILE
4	B	176	PRO
4	B	236	PRO
4	B	272	PRO
4	B	314	VAL
5	L	143	ASP
6	H	57	ASP
3	A	114	ALA
3	A	295	LEU
3	A	324	ASP
3	A	538	ALA
4	B	170	PRO
4	B	211	ARG
4	B	212	TRP
4	B	422	LEU
5	L	28	ASP
5	L	60	SER
5	L	199	LYS
6	H	143	ASN
3	A	135	ILE
3	A	138	GLU
3	A	217	PRO
3	A	302	GLU
3	A	364	ASP
3	A	465	LYS
3	A	485	ALA
3	A	508	ALA
3	A	528	LYS
5	L	78	LEU
3	A	116	PHE
3	A	176	PRO

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Mol	Chain	Res	Type
3	A	458	VAL
4	B	116	PHE
3	A	296	THR
4	B	175	ASN
6	H	10	GLY
3	A	537	PRO
3	A	276	VAL
3	A	421	PRO

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	
3	A	485/498 (97%)	433 (89%)	52 (11%)	6	21
4	B	388/391 (99%)	343 (88%)	45 (12%)	5	18
5	L	190/190 (100%)	168 (88%)	22 (12%)	5	18
6	H	196/196 (100%)	176 (90%)	20 (10%)	7	23
All	All	1259/1275 (99%)	1120 (89%)	139 (11%)	6	20

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	22	LYS
3	A	24	TRP
3	A	27	THR
3	A	49	LYS
3	A	55	PRO
3	A	58	THR
3	A	61	PHE
3	A	65	LYS
3	A	73	LYS
3	A	75	VAL
3	A	80	LEU
3	A	85	GLN
3	A	94	ILE

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Mol	Chain	Res	Type
3	A	101	LYS
3	A	132	ILE
3	A	139	THR
3	A	145	GLN
3	A	199	ARG
3	A	214	LEU
3	A	215	THR
3	A	220	LYS
3	A	221	HIS
3	A	240	THR
3	A	244	ILE
3	A	246	LEU
3	A	263	LYS
3	A	268	SER
3	A	278	GLN
3	A	279	LEU
3	A	290	THR
3	A	325	LEU
3	A	345	PRO
3	A	373	GLN
3	A	376	THR
3	A	385	LYS
3	A	397	THR
3	A	409	THR
3	A	459	THR
3	A	464	GLN
3	A	468	PRO
3	A	469	LEU
3	A	477	THR
3	A	478	GLU
3	A	497	THR
3	A	499	SER
3	A	526	ILE
3	A	533	LEU
3	A	536	VAL
3	A	545	ASN
3	A	547	GLN
3	A	548	VAL
3	A	550	LYS
4	B	2	ILE
4	B	3	SER
4	B	8	VAL

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Mol	Chain	Res	Type
4	B	36	GLU
4	B	55	PRO
4	B	82	LYS
4	B	83	ARG
4	B	100	LEU
4	B	103	LYS
4	B	104	LYS
4	B	106	VAL
4	B	109	LEU
4	B	132	ILE
4	B	148	VAL
4	B	162	SER
4	B	179	VAL
4	B	200	THR
4	B	215	THR
4	B	230	MET
4	B	233	GLU
4	B	234	LEU
4	B	242	GLN
4	B	250	ASP
4	B	257	ILE
4	B	279	LEU
4	B	280	SER
4	B	282	LEU
4	B	286	THR
4	B	295	LEU
4	B	301	LEU
4	B	305	GLU
4	B	318	TYR
4	B	325	LEU
4	B	330	GLN
4	B	332	GLN
4	B	353	LYS
4	B	363	ASN
4	B	386	THR
4	B	395	LYS
4	B	397	THR
4	B	407	GLN
4	B	413	GLU
4	B	419	THR
4	B	422	LEU
4	B	429	LEU

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Mol	Chain	Res	Type
5	L	1	ASP
5	L	7	THR
5	L	15	LEU
5	L	20	THR
5	L	27	GLN
5	L	39	LYS
5	L	41	GLU
5	L	43	THR
5	L	53	SER
5	L	54	LEU
5	L	65	SER
5	L	77	ASN
5	L	83	ILE
5	L	89	GLN
5	L	106	ILE
5	L	116	SER
5	L	126	THR
5	L	138	ASN
5	L	144	ILE
5	L	180	THR
5	L	190	ASN
5	L	203	SER
6	H	11	ILE
6	H	29	LEU
6	H	43	SER
6	H	62	ASN
6	H	64	SER
6	H	72	SER
6	H	84	MET
6	H	94	ILE
6	H	103	THR
6	H	118	SER
6	H	129	PRO
6	H	150	CYS
6	H	157	PRO
6	H	161	THR
6	H	171	SER
6	H	187	LEU
6	H	192	THR
6	H	205	CYS
6	H	206	ASN
6	H	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	GLN
3	A	85	GLN
3	A	145	GLN
3	A	147	ASN
3	A	174	GLN
3	A	197	GLN
3	A	207	GLN
3	A	221	HIS
3	A	222	GLN
3	A	269	GLN
3	A	278	GLN
3	A	306	ASN
3	A	330	GLN
3	A	340	GLN
3	A	343	GLN
3	A	367	GLN
3	A	447	ASN
3	A	464	GLN
3	A	494	ASN
3	A	520	GLN
4	B	96	HIS
4	B	137	ASN
4	B	151	GLN
4	B	161	GLN
4	B	182	GLN
4	B	197	GLN
4	B	235	HIS
4	B	330	GLN
4	B	348	ASN
4	B	363	ASN
4	B	418	ASN
5	L	77	ASN
5	L	89	GLN
5	L	90	GLN
5	L	137	ASN
5	L	138	ASN
5	L	145	ASN
5	L	190	ASN
5	L	210	ASN
6	H	1	GLN
6	H	13	GLN

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Mol	Chain	Res	Type
6	H	59	ASN
6	H	62	ASN
6	H	79	GLN
6	H	83	ASN
6	H	112	HIS
6	H	174	HIS
6	H	206	ASN
6	H	209	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	2DA	P	822	1,2	19,22,23	0.31	0	25,31,34	0.39	0

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
2	2DA	P	822	1,2	-	0/7/18/19	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	822	2DA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	P	3002	-	5,5,5	4.74	5 (100%)	5,5,5	6.13	3 (60%)
7	GOL	B	3001	-	5,5,5	4.65	5 (100%)	5,5,5	6.12	3 (60%)
9	GLC	H	1725	-	12,12,12	0.62	0	17,17,17	0.67	0

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
7	GOL	P	3002	-	-	2/4/4/4	-
7	GOL	B	3001	-	-	2/4/4/4	-
9	GLC	H	1725	-	-	0/2/22/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	3002	GOL	C3-C2	-8.05	1.21	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3001	GOL	C3-C2	-7.77	1.22	1.51
7	B	3001	GOL	O1-C1	4.79	1.62	1.42
7	P	3002	GOL	O1-C1	4.78	1.62	1.42
7	B	3001	GOL	O3-C3	3.42	1.56	1.42
7	P	3002	GOL	O3-C3	3.28	1.56	1.42
7	B	3001	GOL	C1-C2	-2.80	1.41	1.51
7	P	3002	GOL	C1-C2	-2.66	1.41	1.51
7	P	3002	GOL	O2-C2	-2.63	1.35	1.43
7	B	3001	GOL	O2-C2	-2.29	1.36	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	3002	GOL	O3-C3-C2	11.20	160.82	110.38
7	B	3001	GOL	O3-C3-C2	11.13	160.49	110.38
7	B	3001	GOL	O2-C2-C3	7.18	138.92	109.18
7	P	3002	GOL	O2-C2-C3	7.07	138.45	109.18
7	P	3002	GOL	O1-C1-C2	3.40	125.71	110.38
7	B	3001	GOL	O1-C1-C2	3.31	125.30	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	3002	GOL	C1-C2-C3-O3
7	B	3001	GOL	O1-C1-C2-C3
7	B	3001	GOL	C1-C2-C3-O3
7	P	3002	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	H	1725	GLC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	T	24/27 (88%)	0.83	5 (20%) 2 2	43, 87, 120, 126	0
2	P	19/21 (90%)	0.38	1 (5%) 32 24	60, 75, 109, 117	0
3	A	556/558 (99%)	0.48	32 (5%) 29 22	31, 73, 101, 109	1 (0%)
4	B	429/429 (100%)	0.25	22 (5%) 33 25	26, 54, 101, 112	1 (0%)
5	L	211/211 (100%)	0.36	1 (0%) 87 82	39, 64, 98, 104	0
6	H	225/225 (100%)	0.07	7 (3%) 51 41	35, 55, 87, 109	0
All	All	1464/1471 (99%)	0.34	68 (4%) 37 29	26, 63, 101, 126	2 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	429	LEU	7.6
3	A	556	ILE	6.5
6	H	139	ALA	5.9
6	H	138	SER	4.6
6	H	141	GLN	4.2
3	A	1	PRO	4.1
6	H	142	THR	3.9
1	T	703	DG	3.9
6	H	140	ALA	3.8
3	A	448	ARG	3.7
3	A	435	VAL	3.7
4	B	362	THR	3.5
1	T	704	DC	3.5
4	B	314	VAL	3.5
3	A	456	GLY	3.4
2	P	803	DC	3.4
3	A	136	ASN	3.3
4	B	1	PRO	3.3
3	A	102	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	139	THR	3.2
3	A	439	THR	3.2
3	A	223	LYS	3.2
3	A	286	THR	3.2
4	B	357	MET	3.1
3	A	334	GLN	2.9
4	B	422	LEU	2.9
4	B	211	ARG	2.8
3	A	63	ILE	2.8
3	A	434	ILE	2.8
3	A	462	GLY	2.8
4	B	247	PRO	2.6
3	A	494	ASN	2.6
3	A	297	GLU	2.6
3	A	436	GLY	2.5
6	H	143	ASN	2.5
4	B	334	GLN	2.5
6	H	223	ALA	2.5
4	B	354	TYR	2.5
1	T	725	DG	2.5
3	A	66	LYS	2.5
4	B	312	GLU	2.5
3	A	356	ARG	2.4
4	B	243	PRO	2.4
3	A	135	ILE	2.4
4	B	298	GLU	2.4
1	T	702	DT	2.4
3	A	138	GLU	2.4
3	A	252	TRP	2.4
3	A	455	ALA	2.3
4	B	427	TYR	2.3
1	T	705	DA	2.2
3	A	288	ALA	2.2
3	A	69	THR	2.2
4	B	252	TRP	2.2
4	B	318	TYR	2.2
4	B	423	VAL	2.2
3	A	249	LYS	2.2
4	B	88	TRP	2.2
3	A	437	ALA	2.2
4	B	250	ASP	2.1
3	A	426	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	295	LEU	2.1
4	B	315	HIS	2.0
4	B	421	PRO	2.0
5	L	1	ASP	2.0
3	A	529	GLU	2.0
3	A	287	LYS	2.0
3	A	555	GLY	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
2	2DA	P	822	20/21	0.95	0.10	51,54,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	P	3002	6/6	0.79	0.22	62,65,66,68	0
7	GOL	B	3001	6/6	0.83	0.14	67,70,71,72	0
9	GLC	H	1725	12/12	0.85	0.15	61,63,65,67	0
8	MG	A	559	1/1	0.95	0.10	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.