



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:10 AM UTC

PDB ID : 3JSM / pdb_00003jsm
Title : K65R mutant HIV-1 reverse transcriptase cross-linked to DS-DNA and complexed with tenofovir-diphosphate as the incoming nucleotide substrate
Authors : Das, K.; Arnold, E.
Deposited on : 2009-09-10
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

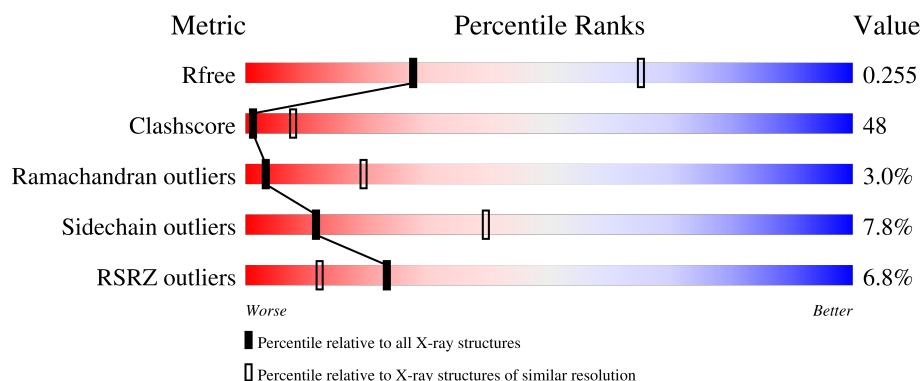
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	4% 15% 52% 22% 11%
2	P	21	5% 19% 48% 29% 5%
3	A	558	3% 35% 56% 8% .
4	B	437	11% 25% 54% 16% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8854 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 DNA (5'-D(*A*TP*GP*GP*TP*CP*GP*GP*CP*GP*C
P*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			

- Molecule 2 is a DNA chain called DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*T
P*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(DDG))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			

- Molecule 3 is a protein called HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	554	Total	C	N	O	S	0	0	0
			4508	2917	751	832	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ARG	LYS	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

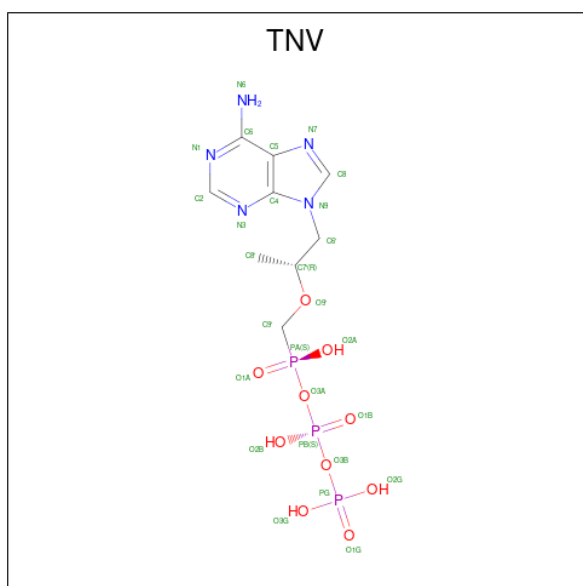
- Molecule 4 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	413	Total	C	N	O	S	0	0	0
			3405	2215	564	620	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
B	430	GLY	-	expression tag	UNP P03366
B	431	GLY	-	expression tag	UNP P03366
B	432	HIS	-	expression tag	UNP P03366
B	433	HIS	-	expression tag	UNP P03366
B	434	HIS	-	expression tag	UNP P03366
B	435	HIS	-	expression tag	UNP P03366
B	436	HIS	-	expression tag	UNP P03366
B	437	HIS	-	expression tag	UNP P03366

- Molecule 5 is [2-(6-AMINO-9H-PURIN-9-YL)-1-METHYLETHOXY]METHYL-TRIPHOSPHATE (CCD ID: TNV) (formula: $C_9H_{16}N_5O_{10}P_3$).

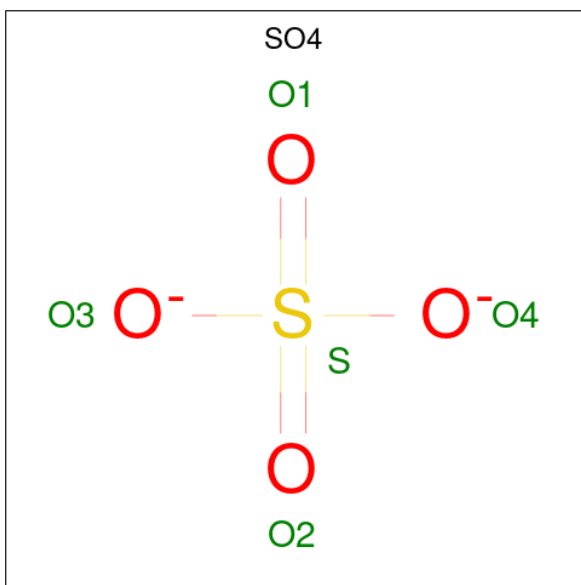


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	9	5	10	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

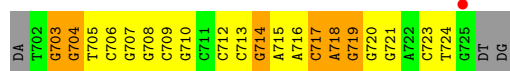
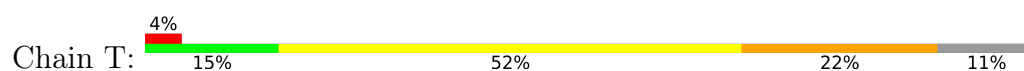
- Molecule 8 is water.

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

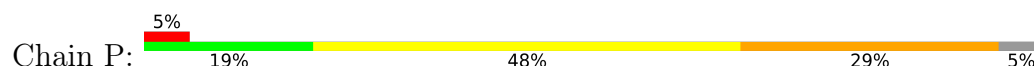
3 Residue-property plots

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

- Molecule 1: DNA (5'-D(*A*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')

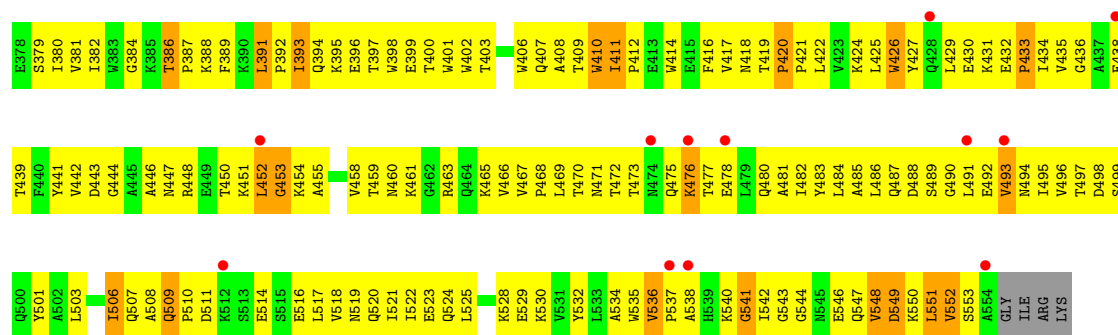


- Molecule 2: DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(DDG))-3')



- Molecule 3: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	170.31Å 170.31Å 155.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.17 – 3.00 49.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.17-3.00) 95.8 (49.17-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.285 0.254 , 0.255	Depositor DCC
R_{free} test set	1482 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: DDG, TNV, MRG, SO4, 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	0.40	0/555	0.99	6/856 (0.7%)
2	P	0.74	1/400 (0.2%)	1.22	6/612 (1.0%)
3	A	0.57	0/4626	1.19	44/6285 (0.7%)
4	B	0.55	0/3502	1.16	38/4760 (0.8%)
All	All	0.56	1/9083 (0.0%)	1.17	94/12513 (0.8%)

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
1	T	0	3
2	P	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	803	DC	O3'-P	-9.12	1.47	1.61

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	241	VAL	N-CA-C	-13.54	91.01	108.89
3	A	3	SER	N-CA-C	11.18	124.16	110.07
3	A	69	THR	N-CA-C	-9.76	101.30	113.01
2	P	806	DT	O5'-P-OP1	-9.51	80.48	109.00
3	A	223	LYS	N-CA-C	-9.48	90.61	110.80
4	B	60	VAL	CB-CA-C	-9.28	98.31	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	84	THR	N-CA-C	-9.02	96.34	109.59
4	B	339	TYR	CB-CA-C	-9.01	94.34	109.48
3	A	219	LYS	N-CA-C	-8.90	91.85	110.80
3	A	552	VAL	CB-CA-C	-8.89	102.20	110.91
3	A	224	GLU	CA-C-N	-8.78	111.34	120.38
3	A	224	GLU	C-N-CA	-8.78	111.34	120.38
4	B	422	LEU	N-CA-C	-8.51	100.57	113.51
3	A	552	VAL	N-CA-C	8.23	119.04	112.12
4	B	423	VAL	N-CA-C	-8.03	104.74	112.29
4	B	51	GLY	CA-C-N	7.83	127.89	119.28
4	B	51	GLY	C-N-CA	7.83	127.89	119.28
2	P	803	DC	O3'-P-O5'	7.75	115.62	104.00
3	A	388	LYS	N-CA-C	-7.57	97.35	109.76
1	T	718	DA	OP2-P-O3'	-7.55	85.36	108.00
1	T	717	DC	OP1-P-O3'	-7.52	85.44	108.00
2	P	805	DG	O3'-P-O5'	7.43	115.14	104.00
1	T	717	DC	P-O3'-C3'	-7.41	109.09	120.20
3	A	222	GLN	N-CA-C	7.35	122.20	111.02
4	B	424	LYS	N-CA-C	-7.31	104.50	113.50
2	P	808	DC	O3'-P-O5'	7.27	114.90	104.00
4	B	68	SER	N-CA-C	-7.26	104.28	113.72
4	B	242	GLN	N-CA-C	-7.20	100.72	109.72
4	B	295	LEU	N-CA-C	6.90	120.67	110.46
3	A	391	LEU	N-CA-C	6.90	120.56	110.14
3	A	411	ILE	CA-C-N	6.86	128.42	119.84
3	A	411	ILE	C-N-CA	6.86	128.42	119.84
3	A	113	ASP	N-CA-C	-6.84	102.00	111.30
4	B	391	LEU	CA-C-N	6.82	128.36	119.84
4	B	391	LEU	C-N-CA	6.82	128.36	119.84
4	B	317	VAL	N-CA-C	6.77	117.88	107.99
3	A	245	VAL	N-CA-C	6.76	118.49	109.37
4	B	408	ALA	CB-CA-C	6.71	120.86	109.53
3	A	386	THR	CA-C-N	6.68	126.64	120.03
3	A	386	THR	C-N-CA	6.68	126.64	120.03
4	B	389	PHE	N-CA-C	6.65	120.13	110.42
3	A	493	VAL	CB-CA-C	-6.53	100.63	110.55
3	A	274	ILE	N-CA-C	-6.53	101.12	109.80
4	B	241	VAL	CB-CA-C	6.52	119.63	111.15
3	A	8	VAL	CA-C-N	6.38	126.60	119.90
3	A	8	VAL	C-N-CA	6.38	126.60	119.90
4	B	390	LYS	N-CA-C	-6.30	97.43	108.20
4	B	408	ALA	N-CA-C	-6.30	100.25	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	320	ASP	CA-C-N	6.27	125.96	119.56
3	A	320	ASP	C-N-CA	6.27	125.96	119.56
3	A	175	ASN	CA-C-N	6.25	126.72	119.47
3	A	175	ASN	C-N-CA	6.25	126.72	119.47
3	A	536	VAL	CA-C-N	6.18	126.54	119.93
3	A	536	VAL	C-N-CA	6.18	126.54	119.93
4	B	147	ASN	N-CA-C	-6.14	106.33	113.88
4	B	5	ILE	N-CA-C	-6.08	96.69	109.34
1	T	719	DG	N9-C1'-C2'	6.00	122.51	113.50
3	A	222	GLN	CB-CA-C	-6.00	103.01	111.65
3	A	290	THR	N-CA-C	-5.99	105.54	114.64
1	T	719	DG	C4'-C3'-O3'	-5.91	101.14	110.00
4	B	131	THR	N-CA-C	5.86	118.45	108.90
4	B	343	GLN	N-CA-C	-5.82	106.72	113.88
4	B	46	LYS	N-CA-C	-5.79	105.31	112.90
4	B	306	ASN	N-CA-C	-5.75	104.87	112.34
4	B	277	ARG	N-CA-C	5.74	120.84	111.37
3	A	452	LEU	N-CA-C	5.71	118.69	109.79
4	B	338	THR	N-CA-C	5.68	118.80	109.72
3	A	360	ALA	N-CA-C	-5.65	107.39	114.56
3	A	549	ASP	CB-CA-C	-5.63	101.44	110.79
3	A	366	LYS	N-CA-C	-5.58	105.10	111.07
3	A	506	ILE	N-CA-C	5.58	118.02	111.05
2	P	805	DG	OP1-P-O3'	5.56	124.67	108.00
3	A	453	GLY	N-CA-C	-5.53	102.12	111.08
4	B	65	LYS	N-CA-C	5.52	118.42	108.48
3	A	410	TRP	N-CA-C	5.52	117.46	109.07
4	B	413	GLU	N-CA-C	-5.49	103.45	110.53
3	A	303	LEU	N-CA-C	-5.48	104.94	111.03
4	B	55	PRO	N-CA-C	5.47	120.37	114.68
2	P	808	DC	P-O3'-C3'	-5.45	112.02	120.20
3	A	214	LEU	N-CA-C	5.41	117.34	108.52
3	A	37	ILE	CB-CA-C	-5.38	104.99	112.04
3	A	92	LEU	N-CA-C	5.33	119.42	113.02
4	B	409	THR	N-CA-C	-5.32	107.34	112.97
3	A	381	VAL	CB-CA-C	-5.30	105.10	112.04
4	B	275	LYS	N-CA-C	5.24	118.04	110.28
4	B	391	LEU	N-CA-C	5.20	117.15	110.39
3	A	28	GLU	N-CA-C	-5.19	106.90	113.18
4	B	24	TRP	CA-C-N	5.12	126.24	119.84
4	B	24	TRP	C-N-CA	5.12	126.24	119.84
4	B	301	LEU	N-CA-C	-5.11	106.20	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	719	DG	C2'-C3'-O3'	5.07	119.11	111.50
4	B	211	ARG	N-CA-C	-5.03	107.64	112.97
3	A	256	ASP	N-CA-C	-5.03	105.71	111.14
3	A	287	LYS	N-CA-C	5.03	115.68	108.74

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	815	DG	Sidechain
1	T	703	DG	Sidechain
1	T	704	DG	Sidechain
1	T	714	DG	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	494	0	269	34	0
2	P	407	0	231	35	0
3	A	4508	0	4566	414	0
4	B	3405	0	3437	395	0
5	A	27	0	12	1	0
6	A	2	0	0	0	0
7	A	10	0	0	0	0
8	A	1	0	0	0	0
All	All	8854	0	8515	822	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 48.

All (822) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:195:ILE:HD11	3:A:199:ARG:HE	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:332:GLN:HB2	4:B:336:GLN:HB3	1.33	1.08
3:A:408:ALA:HB1	4:B:364:ASP:HB3	1.39	1.04
3:A:195:ILE:HD11	3:A:199:ARG:NE	1.76	1.01
4:B:246:LEU:HD22	4:B:260:LEU:HD11	1.47	0.97
3:A:484:LEU:HA	3:A:487:GLN:HE21	1.26	0.97
4:B:363:ASN:HD21	4:B:365:VAL:HG22	1.31	0.94
3:A:195:ILE:CD1	3:A:199:ARG:HE	1.81	0.93
3:A:195:ILE:HG23	3:A:196:GLY:N	1.84	0.92
4:B:13:LYS:HG3	4:B:85:GLN:HA	1.49	0.91
3:A:28:GLU:HG3	3:A:135:ILE:HG12	1.51	0.91
4:B:303:LEU:O	4:B:307:ARG:HB2	1.71	0.90
3:A:434:ILE:HD13	3:A:530:LYS:HB3	1.53	0.90
3:A:191:SER:HB3	3:A:198:HIS:HD1	1.37	0.90
4:B:167:ILE:HG23	4:B:212:TRP:CE3	2.07	0.90
2:P:817:MRG:N3	2:P:817:MRG:H221	1.84	0.89
4:B:21:VAL:CG1	4:B:59:PRO:HD3	2.03	0.89
2:P:808:DC:H2''	3:A:475:GLN:OE1	1.73	0.88
4:B:134:SER:OG	4:B:139:THR:HG23	1.74	0.88
3:A:452:LEU:HG	3:A:470:THR:HA	1.55	0.87
1:T:720:DG:H2'	1:T:721:DG:C8	2.10	0.87
4:B:56:TYR:HE2	4:B:126:LYS:HE3	1.39	0.86
4:B:270:ILE:HG23	4:B:271:TYR:CD1	2.11	0.85
3:A:354:TYR:HD2	3:A:371:ALA:HB2	1.40	0.85
3:A:420:PRO:HA	3:A:421:PRO:C	2.02	0.85
3:A:447:ASN:ND2	3:A:450:THR:HG23	1.92	0.84
4:B:122:GLU:HA	4:B:125:ARG:HD2	1.57	0.84
4:B:85:GLN:C	4:B:87:PHE:H	1.83	0.83
3:A:406:TRP:CD1	3:A:407:GLN:HG3	2.14	0.83
4:B:103:LYS:HE2	4:B:103:LYS:HA	1.58	0.82
3:A:509:GLN:N	3:A:510:PRO:HD3	1.93	0.82
3:A:343:GLN:HG3	3:A:349:LEU:HD11	1.62	0.81
4:B:209:LEU:HD22	4:B:214:LEU:HD12	1.63	0.81
4:B:64:LYS:HE2	4:B:69:THR:HA	1.63	0.80
4:B:302:GLU:HG2	4:B:306:ASN:ND2	1.97	0.79
3:A:195:ILE:CG2	3:A:196:GLY:H	1.94	0.79
3:A:60:VAL:HG12	3:A:75:VAL:HG13	1.64	0.79
3:A:447:ASN:HB3	3:A:450:THR:OG1	1.82	0.79
3:A:547:GLN:O	3:A:551:LEU:HG	1.82	0.79
3:A:317:VAL:HG12	3:A:318:TYR:H	1.46	0.79
3:A:191:SER:HB3	3:A:198:HIS:ND1	1.96	0.78
4:B:246:LEU:HD22	4:B:260:LEU:CD1	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:195:ILE:CG2	3:A:196:GLY:N	2.46	0.78
4:B:278:GLN:HB2	4:B:302:GLU:OE2	1.83	0.77
4:B:93:GLY:O	4:B:94:ILE:HD12	1.83	0.77
1:T:723:DC:H2'	1:T:724:DT:C6	2.19	0.77
4:B:253:THR:OG1	4:B:256:ASP:HB2	1.85	0.77
4:B:21:VAL:HG11	4:B:59:PRO:HD3	1.67	0.77
3:A:447:ASN:HD22	3:A:450:THR:HG23	1.47	0.76
4:B:356:ARG:HD2	4:B:361:HIS:HA	1.68	0.76
2:P:822:DDG:H5'	3:A:230:MET:HE1	1.64	0.76
3:A:138:GLU:HG3	3:A:139:THR:H	1.52	0.75
4:B:413:GLU:HG2	4:B:414:TRP:N	2.00	0.75
3:A:94:ILE:CG2	3:A:95:PRO:HD2	2.17	0.75
4:B:21:VAL:HG13	4:B:59:PRO:HD3	1.67	0.75
3:A:444:GLY:HA2	3:A:552:VAL:HG11	1.67	0.75
4:B:175:ASN:N	4:B:176:PRO:HD3	2.01	0.75
3:A:96:HIS:CD2	3:A:97:PRO:HD2	2.21	0.74
4:B:363:ASN:ND2	4:B:365:VAL:HG22	2.02	0.74
4:B:112:GLY:C	4:B:114:ALA:H	1.93	0.74
4:B:332:GLN:HE22	4:B:424:LYS:HB3	1.53	0.74
3:A:195:ILE:HG23	3:A:196:GLY:H	1.46	0.74
3:A:224:GLU:O	3:A:225:PRO:C	2.30	0.74
1:T:714:DG:H4'	3:A:286:THR:HG21	1.70	0.74
4:B:363:ASN:HD21	4:B:365:VAL:CG2	2.01	0.74
2:P:804:DA:H2''	2:P:805:DG:OP1	1.88	0.73
2:P:806:DT:O2	3:A:448:ARG:NH2	2.21	0.73
3:A:221:HIS:CE1	3:A:228:LEU:H	2.06	0.73
3:A:220:LYS:O	3:A:220:LYS:HG2	1.88	0.73
4:B:335:GLY:O	4:B:355:ALA:HA	1.89	0.73
3:A:503:LEU:HD22	3:A:535:TRP:HB2	1.71	0.73
4:B:154:LYS:O	4:B:157:PRO:HD2	1.87	0.72
3:A:394:GLN:HB2	3:A:397:THR:OG1	1.89	0.72
3:A:195:ILE:HG13	3:A:199:ARG:HD2	1.71	0.72
3:A:459:THR:CG2	3:A:463:ARG:HB3	2.19	0.72
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.23	0.72
3:A:88:TRP:HB3	4:B:143:ARG:NH1	2.04	0.72
3:A:254:VAL:HG13	3:A:283:LEU:HD22	1.70	0.72
3:A:443:ASP:OD2	3:A:444:GLY:N	2.20	0.72
3:A:181:TYR:HE2	4:B:136:ASN:HD22	1.38	0.72
3:A:94:ILE:HG22	3:A:95:PRO:HD2	1.72	0.71
3:A:441:TYR:HA	3:A:496:VAL:HG12	1.72	0.71
4:B:426:TRP:N	4:B:426:TRP:CD1	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:85:GLN:C	4:B:87:PHE:N	2.46	0.71
4:B:395:LYS:HG3	4:B:416:PHE:CE2	2.24	0.71
3:A:478:GLU:HG2	3:A:499:SER:HB3	1.72	0.71
3:A:135:ILE:C	3:A:137:ASN:H	1.97	0.71
4:B:81:ASN:HA	4:B:84:THR:HG22	1.71	0.71
4:B:100:LEU:HD23	4:B:103:LYS:HG3	1.71	0.71
4:B:164:MET:HA	4:B:167:ILE:HD12	1.72	0.71
4:B:109:LEU:HG	4:B:216:THR:HG21	1.72	0.71
3:A:220:LYS:HE3	3:A:222:GLN:HG2	1.73	0.70
4:B:206:ARG:HB3	4:B:206:ARG:NH1	2.06	0.70
4:B:104:LYS:HG2	4:B:192:ASP:OD1	1.91	0.70
3:A:532:TYR:HE2	3:A:534:ALA:HB2	1.56	0.70
1:T:714:DG:H4'	3:A:286:THR:CG2	2.21	0.70
4:B:254:VAL:HG12	4:B:258:GLN:OE1	1.91	0.70
3:A:317:VAL:HG12	3:A:318:TYR:N	2.05	0.70
3:A:34:LEU:HD11	3:A:62:ALA:HB2	1.74	0.70
3:A:546:GLU:HA	3:A:549:ASP:OD2	1.92	0.70
4:B:325:LEU:O	4:B:387:PRO:HA	1.92	0.70
4:B:395:LYS:HE2	4:B:399:GLU:OE2	1.92	0.70
3:A:337:TRP:CZ3	3:A:368:LEU:HD13	2.27	0.69
4:B:395:LYS:HG2	4:B:399:GLU:OE1	1.91	0.69
4:B:100:LEU:HA	4:B:103:LYS:HG2	1.74	0.69
4:B:282:LEU:CD2	4:B:295:LEU:HD23	2.23	0.69
2:P:803:DC:H2''	2:P:804:DA:OP1	1.93	0.69
3:A:198:HIS:NE2	3:A:202:ILE:HD13	2.08	0.69
4:B:240:THR:HG22	4:B:241:VAL:O	1.92	0.69
4:B:282:LEU:HD12	4:B:282:LEU:H	1.58	0.69
2:P:817:MRG:N3	2:P:817:MRG:C22	2.45	0.68
3:A:470:THR:HG22	3:A:471:ASN:ND2	2.08	0.68
4:B:154:LYS:NZ	4:B:184:MET:HE1	2.07	0.68
3:A:340:GLN:HB3	3:A:351:THR:HG22	1.75	0.68
4:B:365:VAL:HG12	4:B:393:ILE:CD1	2.23	0.68
3:A:408:ALA:CB	4:B:364:ASP:HB3	2.21	0.68
3:A:92:LEU:CD1	4:B:133:PRO:HB3	2.23	0.68
3:A:503:LEU:O	3:A:507:GLN:HG3	1.93	0.68
4:B:167:ILE:HA	4:B:212:TRP:CZ3	2.28	0.68
4:B:344:GLU:OE1	4:B:344:GLU:HA	1.93	0.68
3:A:105:SER:HB2	3:A:198:HIS:ND1	2.09	0.68
3:A:532:TYR:CE2	3:A:534:ALA:HB2	2.27	0.68
3:A:31:ILE:O	3:A:35:VAL:HG23	1.93	0.68
4:B:422:LEU:HA	4:B:425:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:508:ALA:C	3:A:510:PRO:HD3	2.18	0.68
1:T:719:DG:H2''	1:T:720:DG:O5'	1.93	0.68
3:A:56:TYR:O	3:A:143:ARG:NH2	2.27	0.68
4:B:13:LYS:HB3	4:B:14:PRO:HD2	1.76	0.68
4:B:40:GLU:OE1	4:B:40:GLU:HA	1.93	0.68
3:A:417:VAL:O	3:A:417:VAL:HG13	1.93	0.67
4:B:178:ILE:HD11	4:B:201:LYS:NZ	2.09	0.67
3:A:484:LEU:HA	3:A:487:GLN:NE2	2.06	0.67
3:A:395:LYS:HE3	3:A:414:TRP:NE1	2.10	0.67
3:A:408:ALA:HB2	4:B:337:TRP:HH2	1.60	0.67
3:A:244:ILE:HD13	3:A:267:ALA:HB2	1.77	0.67
4:B:331:LYS:NZ	4:B:364:ASP:OD1	2.27	0.66
3:A:391:LEU:HD12	3:A:414:TRP:CE3	2.30	0.66
4:B:120:LEU:HD12	4:B:121:ASP:N	2.10	0.66
4:B:85:GLN:O	4:B:87:PHE:N	2.28	0.66
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.29	0.66
4:B:154:LYS:HZ1	4:B:184:MET:HE1	1.60	0.66
4:B:326:ILE:HG22	4:B:327:ALA:H	1.59	0.66
3:A:469:LEU:HD12	3:A:477:THR:HG22	1.77	0.66
3:A:226:PRO:HB3	3:A:235:HIS:CD2	2.30	0.66
3:A:273:GLY:H	3:A:338:THR:HG21	1.61	0.66
3:A:478:GLU:O	3:A:482:ILE:HG13	1.95	0.66
3:A:92:LEU:HD12	4:B:133:PRO:HB3	1.77	0.66
4:B:169:GLU:CG	4:B:170:PRO:HD3	2.25	0.66
4:B:334:GLN:O	4:B:334:GLN:HG2	1.94	0.66
4:B:80:LEU:O	4:B:83:ARG:N	2.28	0.65
4:B:421:PRO:C	4:B:423:VAL:H	2.04	0.65
3:A:181:TYR:HE2	4:B:136:ASN:ND2	1.92	0.65
4:B:376:THR:HG1	4:B:389:PHE:HZ	1.45	0.65
3:A:281:LYS:O	3:A:284:ARG:HG3	1.96	0.65
3:A:395:LYS:HE3	3:A:414:TRP:CE2	2.32	0.65
3:A:221:HIS:HE1	3:A:228:LEU:HB2	1.62	0.64
3:A:447:ASN:HD22	3:A:450:THR:H	1.45	0.64
3:A:105:SER:HB2	3:A:198:HIS:HD1	1.62	0.64
4:B:343:GLN:HG3	4:B:349:LEU:HD11	1.78	0.64
1:T:706:DC:H2'	1:T:707:DG:C8	2.33	0.64
4:B:426:TRP:CD1	4:B:426:TRP:H	2.16	0.64
3:A:282:LEU:HD21	3:A:295:LEU:HD23	1.79	0.63
2:P:822:DDG:H5'	3:A:230:MET:CE	2.27	0.63
3:A:252:TRP:HZ3	3:A:260:LEU:HD13	1.61	0.63
4:B:421:PRO:HB3	4:B:424:LYS:HE3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:178:ILE:HD11	4:B:201:LYS:HD3	1.80	0.63
4:B:417:VAL:HG22	4:B:419:THR:HG23	1.81	0.63
4:B:266:TRP:HB3	4:B:426:TRP:CH2	2.34	0.63
3:A:288:ALA:C	3:A:290:THR:H	2.07	0.63
4:B:85:GLN:CG	4:B:86:ASP:N	2.61	0.63
3:A:118:VAL:HB	3:A:149:LEU:HD12	1.80	0.63
4:B:413:GLU:CG	4:B:414:TRP:N	2.61	0.63
2:P:805:DG:C2'	2:P:806:DT:O5'	2.47	0.62
3:A:395:LYS:HD2	3:A:414:TRP:CZ2	2.34	0.62
4:B:3:SER:N	4:B:4:PRO:HD3	2.13	0.62
3:A:254:VAL:HG13	3:A:283:LEU:CD2	2.29	0.62
3:A:354:TYR:CD2	3:A:371:ALA:HB2	2.28	0.62
3:A:516:GLU:O	3:A:520:GLN:HG3	2.00	0.62
3:A:459:THR:HG23	3:A:463:ARG:HB3	1.81	0.62
3:A:509:GLN:N	3:A:510:PRO:CD	2.63	0.62
3:A:95:PRO:HA	4:B:136:ASN:O	2.00	0.62
4:B:56:TYR:CE2	4:B:126:LYS:HE3	2.29	0.62
4:B:363:ASN:O	4:B:367:GLN:HG3	1.98	0.62
3:A:368:LEU:O	3:A:372:VAL:HG23	1.99	0.62
4:B:85:GLN:CG	4:B:86:ASP:H	2.13	0.62
3:A:21:VAL:HG13	3:A:59:PRO:HD3	1.82	0.62
4:B:178:ILE:CD1	4:B:201:LYS:HD3	2.30	0.62
4:B:240:THR:HG22	4:B:241:VAL:N	2.14	0.62
4:B:339:TYR:HB2	4:B:352:GLY:N	2.15	0.62
4:B:13:LYS:N	4:B:85:GLN:HB2	2.15	0.61
4:B:246:LEU:HB3	4:B:247:PRO:HD2	1.81	0.61
4:B:326:ILE:HG22	4:B:327:ALA:N	2.15	0.61
4:B:361:HIS:CD2	4:B:361:HIS:H	2.16	0.61
3:A:255:ASN:HA	3:A:258:CYS:SG	2.40	0.61
4:B:244:ILE:HG13	4:B:426:TRP:O	2.01	0.61
4:B:276:VAL:HG13	4:B:277:ARG:H	1.66	0.61
1:T:712:DC:H2'	1:T:713:DC:C6	2.35	0.61
4:B:330:GLN:HB2	4:B:338:THR:OG1	2.01	0.61
3:A:244:ILE:HG12	3:A:244:ILE:O	1.99	0.61
4:B:339:TYR:HE2	4:B:378:GLU:OE1	1.83	0.61
3:A:41:MET:HE2	3:A:46:LYS:HB2	1.82	0.60
3:A:59:PRO:HG2	3:A:76:ASP:HB3	1.83	0.60
4:B:169:GLU:HG3	4:B:170:PRO:HD3	1.83	0.60
4:B:85:GLN:HG3	4:B:86:ASP:H	1.65	0.60
3:A:376:THR:O	3:A:377:THR:C	2.44	0.60
4:B:282:LEU:HD21	4:B:295:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:395:LYS:HE2	4:B:399:GLU:CD	2.26	0.60
2:P:812:DT:H2'	2:P:813:DT:C6	2.36	0.60
3:A:107:THR:HG21	3:A:202:ILE:HG12	1.82	0.60
4:B:112:GLY:C	4:B:114:ALA:N	2.56	0.60
4:B:406:TRP:O	4:B:407:GLN:HG3	2.00	0.60
3:A:63:ILE:HG22	3:A:64:LYS:N	2.17	0.60
3:A:484:LEU:C	3:A:486:LEU:H	2.09	0.60
4:B:104:LYS:HB2	4:B:192:ASP:HA	1.84	0.60
4:B:97:PRO:O	4:B:99:GLY:N	2.35	0.60
4:B:118:VAL:O	4:B:119:PRO:C	2.45	0.60
3:A:277:ARG:NH2	3:A:355:ALA:O	2.34	0.59
4:B:330:GLN:CD	4:B:340:GLN:HE22	2.10	0.59
3:A:446:ALA:CB	3:A:453:GLY:HA3	2.32	0.59
4:B:125:ARG:HG2	4:B:146:TYR:O	2.02	0.59
3:A:68:SER:C	3:A:70:LYS:H	2.11	0.59
3:A:118:VAL:HB	3:A:149:LEU:CD1	2.31	0.59
3:A:271:TYR:CE1	3:A:314:VAL:HG22	2.37	0.59
4:B:339:TYR:HB2	4:B:352:GLY:H	1.67	0.59
3:A:452:LEU:HB3	3:A:469:LEU:O	2.02	0.59
4:B:266:TRP:C	4:B:268:SER:H	2.09	0.59
3:A:181:TYR:CE2	4:B:136:ASN:ND2	2.69	0.59
3:A:426:TRP:CE3	3:A:426:TRP:HA	2.37	0.59
3:A:535:TRP:HB3	4:B:422:LEU:CD2	2.33	0.59
4:B:348:ASN:HD22	4:B:351:THR:HG22	1.67	0.59
3:A:529:GLU:O	3:A:530:LYS:HG3	2.03	0.59
4:B:134:SER:HG	4:B:139:THR:HG23	1.68	0.59
4:B:210:LEU:HD12	4:B:210:LEU:C	2.27	0.59
3:A:195:ILE:CD1	3:A:199:ARG:NE	2.53	0.58
3:A:454:LYS:HG3	3:A:552:VAL:HG13	1.84	0.58
4:B:319:TYR:O	4:B:321:PRO:HD3	2.02	0.58
2:P:805:DG:H21	3:A:448:ARG:HH12	1.50	0.58
3:A:244:ILE:CD1	3:A:267:ALA:HB2	2.33	0.58
3:A:218:ASP:OD1	3:A:218:ASP:N	2.37	0.58
3:A:455:ALA:HB1	3:A:481:ALA:HB2	1.84	0.58
3:A:33:ALA:O	3:A:37:ILE:HG13	2.03	0.58
4:B:8:VAL:HG21	4:B:159:ILE:HG12	1.85	0.58
3:A:487:GLN:HG3	3:A:488:ASP:OD1	2.02	0.58
4:B:246:LEU:HD21	4:B:264:LEU:HD21	1.84	0.58
4:B:345:PRO:O	4:B:346:PHE:HB2	2.03	0.58
3:A:23:GLN:NE2	3:A:59:PRO:HA	2.18	0.58
3:A:336:GLN:C	3:A:337:TRP:CD1	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:475:GLN:HB3	3:A:501:TYR:CD2	2.38	0.58
4:B:86:ASP:O	4:B:89:GLU:N	2.32	0.58
4:B:13:LYS:HG3	4:B:85:GLN:CA	2.28	0.58
4:B:273:GLY:O	4:B:309:ILE:HD13	2.04	0.57
2:P:805:DG:H2''	2:P:806:DT:O5'	2.03	0.57
3:A:426:TRP:HA	3:A:426:TRP:HE3	1.69	0.57
4:B:277:ARG:HA	4:B:280:SER:HB3	1.86	0.57
3:A:58:THR:HG23	3:A:59:PRO:HD2	1.86	0.57
3:A:475:GLN:C	3:A:477:THR:H	2.13	0.57
1:T:720:DG:H1	2:P:808:DC:N4	2.02	0.57
4:B:122:GLU:HA	4:B:125:ARG:CD	2.34	0.57
4:B:163:SER:O	4:B:167:ILE:HG13	2.05	0.57
4:B:270:ILE:HG23	4:B:271:TYR:HD1	1.62	0.57
3:A:484:LEU:O	3:A:486:LEU:N	2.38	0.57
3:A:497:THR:O	3:A:535:TRP:HA	2.05	0.57
4:B:274:ILE:HG13	4:B:309:ILE:HD12	1.86	0.57
3:A:342:TYR:HB3	3:A:348:ASN:HB3	1.86	0.56
3:A:430:GLU:OE2	3:A:530:LYS:HG2	2.05	0.56
3:A:253:THR:O	3:A:257:ILE:HG12	2.05	0.56
3:A:394:GLN:C	3:A:396:GLU:H	2.14	0.56
4:B:24:TRP:HH2	4:B:61:PHE:CE1	2.22	0.56
3:A:441:TYR:HA	3:A:496:VAL:CG1	2.33	0.56
4:B:167:ILE:HG23	4:B:212:TRP:HE3	1.64	0.56
4:B:330:GLN:O	4:B:337:TRP:HA	2.04	0.56
2:P:804:DA:H2'	2:P:805:DG:C8	2.40	0.56
3:A:207:GLN:HB3	3:A:211:ARG:HH21	1.70	0.56
4:B:209:LEU:HD22	4:B:214:LEU:CD1	2.34	0.56
4:B:278:GLN:OE1	4:B:298:GLU:HB2	2.06	0.56
3:A:521:ILE:O	3:A:525:LEU:HG	2.05	0.56
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.87	0.56
4:B:118:VAL:HB	4:B:149:LEU:HD12	1.87	0.56
3:A:47:ILE:HG22	3:A:146:TYR:HA	1.88	0.56
3:A:68:SER:C	3:A:70:LYS:N	2.61	0.56
3:A:254:VAL:HB	3:A:289:LEU:HA	1.86	0.56
4:B:120:LEU:HD12	4:B:121:ASP:H	1.71	0.56
3:A:91:GLN:HB2	3:A:161:GLN:HE22	1.71	0.56
3:A:342:TYR:HA	3:A:349:LEU:HD12	1.87	0.56
3:A:230:MET:HA	3:A:230:MET:HE2	1.86	0.56
3:A:493:VAL:HG12	3:A:494:ASN:N	2.21	0.56
4:B:64:LYS:HE2	4:B:69:THR:CA	2.35	0.56
3:A:5:ILE:HD13	3:A:163:SER:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:363:ASN:O	3:A:367:GLN:HG3	2.06	0.55
3:A:549:ASP:O	3:A:553:SER:N	2.30	0.55
4:B:266:TRP:CE3	4:B:426:TRP:HH2	2.23	0.55
2:P:816:DG:H2'	2:P:817:MRG:H8	1.88	0.55
3:A:305:GLU:O	3:A:308:GLU:HB2	2.06	0.55
3:A:447:ASN:ND2	3:A:450:THR:H	2.03	0.55
3:A:447:ASN:HD22	3:A:450:THR:CG2	2.19	0.55
4:B:81:ASN:HA	4:B:84:THR:CG2	2.36	0.55
4:B:348:ASN:HD22	4:B:351:THR:CG2	2.20	0.55
3:A:362:THR:HB	3:A:366:LYS:HD2	1.88	0.55
3:A:298:GLU:H	3:A:298:GLU:CD	2.14	0.55
3:A:454:LYS:HE3	3:A:552:VAL:HA	1.88	0.55
4:B:328:GLU:HG3	4:B:342:TYR:HE2	1.72	0.55
3:A:482:ILE:O	3:A:486:LEU:HG	2.07	0.55
3:A:548:VAL:O	3:A:552:VAL:HG23	2.07	0.55
4:B:100:LEU:HA	4:B:103:LYS:CG	2.37	0.55
4:B:282:LEU:HD12	4:B:282:LEU:N	2.22	0.54
4:B:314:VAL:HG22	4:B:315:HIS:N	2.22	0.54
4:B:270:ILE:HG13	4:B:270:ILE:O	2.07	0.54
2:P:817:MRG:H4'	3:A:289:LEU:HD21	1.87	0.54
2:P:805:DG:N2	3:A:448:ARG:HH22	2.06	0.54
4:B:103:LYS:HD3	4:B:190:GLY:C	2.33	0.54
4:B:413:GLU:HG2	4:B:414:TRP:H	1.71	0.54
1:T:708:DG:H2'	1:T:709:DC:C6	2.43	0.54
4:B:178:ILE:HD11	4:B:201:LYS:CD	2.37	0.54
4:B:307:ARG:HG2	4:B:307:ARG:HH11	1.73	0.54
4:B:388:LYS:O	4:B:388:LYS:CD	2.55	0.54
3:A:188:TYR:CD1	3:A:188:TYR:C	2.86	0.54
4:B:183:TYR:CE2	4:B:184:MET:HE2	2.42	0.54
3:A:399:GLU:HA	3:A:402:TRP:CD1	2.42	0.53
3:A:452:LEU:HG	3:A:470:THR:CA	2.34	0.53
3:A:358:ARG:HH21	3:A:370:GLU:HG2	1.72	0.53
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.90	0.53
3:A:198:HIS:C	3:A:198:HIS:CD2	2.87	0.53
4:B:180:ILE:HG12	4:B:189:VAL:HG13	1.91	0.53
3:A:382:ILE:HA	4:B:136:ASN:HA	1.89	0.53
3:A:543:GLY:HA3	4:B:283:LEU:HD12	1.90	0.53
4:B:375:ILE:HG12	4:B:389:PHE:CZ	2.44	0.53
3:A:24:TRP:HZ3	3:A:26:LEU:HD21	1.74	0.53
3:A:193:LEU:HB2	3:A:198:HIS:HB2	1.91	0.53
3:A:439:THR:HG21	4:B:289:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:365:VAL:HG12	4:B:393:ILE:HD12	1.89	0.53
1:T:708:DG:H5'	3:A:89:GLU:HG3	1.91	0.52
4:B:254:VAL:HB	4:B:289:LEU:HA	1.89	0.52
3:A:221:HIS:HE1	3:A:228:LEU:H	1.53	0.52
4:B:422:LEU:HD12	4:B:425:LEU:HD11	1.90	0.52
3:A:27:THR:O	3:A:31:ILE:HG13	2.09	0.52
3:A:94:ILE:HG23	3:A:95:PRO:HD2	1.89	0.52
3:A:38:CYS:SG	3:A:132:ILE:HD11	2.50	0.52
3:A:135:ILE:C	3:A:137:ASN:N	2.63	0.52
3:A:391:LEU:HB3	3:A:393:ILE:HG22	1.90	0.52
4:B:41:MET:HB3	4:B:47:ILE:HG12	1.91	0.52
4:B:169:GLU:HG3	4:B:170:PRO:CD	2.40	0.52
4:B:174:GLN:NE2	4:B:175:ASN:OD1	2.42	0.52
4:B:125:ARG:NE	4:B:147:ASN:HA	2.24	0.52
1:T:708:DG:H21	3:A:94:ILE:HD11	1.74	0.52
3:A:279:LEU:HB2	3:A:302:GLU:OE2	2.10	0.52
4:B:307:ARG:HG2	4:B:307:ARG:NH1	2.25	0.52
3:A:257:ILE:O	3:A:261:VAL:HG23	2.09	0.52
3:A:317:VAL:CG1	3:A:318:TYR:H	2.20	0.52
3:A:517:LEU:HD22	3:A:521:ILE:HD11	1.92	0.52
4:B:97:PRO:C	4:B:99:GLY:H	2.18	0.52
4:B:413:GLU:CG	4:B:414:TRP:H	2.21	0.52
2:P:810:DT:OP1	3:A:361:HIS:NE2	2.41	0.52
3:A:92:LEU:HD12	4:B:133:PRO:CB	2.40	0.52
4:B:175:ASN:N	4:B:176:PRO:CD	2.72	0.52
4:B:339:TYR:O	4:B:351:THR:HB	2.10	0.52
3:A:396:GLU:O	3:A:397:THR:C	2.52	0.52
2:P:805:DG:C6	2:P:806:DT:C4	2.98	0.51
4:B:279:LEU:HA	4:B:282:LEU:HD13	1.91	0.51
3:A:397:THR:HG21	3:A:424:LYS:HA	1.92	0.51
4:B:93:GLY:C	4:B:94:ILE:HD12	2.35	0.51
4:B:304:ALA:HA	4:B:307:ARG:HD3	1.93	0.51
3:A:344:GLU:OE1	3:A:344:GLU:HA	2.10	0.51
4:B:136:ASN:O	4:B:136:ASN:CG	2.54	0.51
4:B:317:VAL:HG23	4:B:317:VAL:O	2.10	0.51
3:A:432:GLU:OE2	3:A:433:PRO:HD2	2.09	0.51
4:B:268:SER:O	4:B:271:TYR:C	2.54	0.51
4:B:332:GLN:HA	4:B:332:GLN:OE1	2.11	0.51
4:B:240:THR:HG22	4:B:241:VAL:H	1.74	0.51
4:B:305:GLU:C	4:B:307:ARG:N	2.65	0.51
3:A:105:SER:CB	3:A:198:HIS:ND1	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:720:DG:H1	2:P:808:DC:H42	1.58	0.51
3:A:255:ASN:HB3	3:A:289:LEU:HB3	1.93	0.51
3:A:380:ILE:O	3:A:384:GLY:N	2.44	0.51
4:B:27:THR:HG22	4:B:28:GLU:N	2.26	0.51
4:B:94:ILE:HG21	4:B:181:TYR:HE1	1.76	0.51
4:B:239:TRP:CH2	4:B:353:LYS:O	2.63	0.51
3:A:226:PRO:HB3	3:A:235:HIS:NE2	2.26	0.51
4:B:246:LEU:HD23	4:B:263:LYS:HE2	1.92	0.51
4:B:374:LYS:O	4:B:378:GLU:HG3	2.11	0.51
4:B:108:VAL:HG22	4:B:188:TYR:CD2	2.46	0.51
4:B:266:TRP:CE3	4:B:426:TRP:CH2	2.98	0.51
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.45	0.51
3:A:447:ASN:HB3	3:A:450:THR:HG1	1.72	0.50
3:A:475:GLN:C	3:A:477:THR:N	2.69	0.50
3:A:480:GLN:O	3:A:483:TYR:HB3	2.10	0.50
3:A:484:LEU:C	3:A:486:LEU:N	2.69	0.50
4:B:112:GLY:O	4:B:114:ALA:N	2.44	0.50
4:B:390:LYS:HD2	4:B:415:GLU:OE2	2.11	0.50
3:A:280:SER:O	3:A:283:LEU:N	2.44	0.50
3:A:369:THR:CG2	3:A:411:ILE:HD11	2.42	0.50
3:A:438:GLU:OE2	3:A:461:LYS:HE2	2.12	0.50
4:B:303:LEU:O	4:B:303:LEU:HD12	2.11	0.50
3:A:333:GLY:O	3:A:334:GLN:HG2	2.12	0.50
3:A:446:ALA:HA	3:A:453:GLY:HA3	1.92	0.50
4:B:333:GLY:O	4:B:336:GLN:HB2	2.10	0.50
4:B:389:PHE:HD1	4:B:389:PHE:H	1.59	0.50
3:A:24:TRP:CZ3	3:A:26:LEU:HD21	2.46	0.50
4:B:111:VAL:O	4:B:113:ASP:N	2.44	0.50
4:B:259:LYS:O	4:B:261:VAL:N	2.44	0.50
3:A:335:GLY:O	3:A:337:TRP:CD1	2.65	0.50
3:A:434:ILE:HB	3:A:494:ASN:HD21	1.76	0.50
3:A:24:TRP:CE3	3:A:24:TRP:O	2.65	0.50
4:B:206:ARG:HB3	4:B:206:ARG:HH11	1.77	0.50
2:P:809:DC:H2''	2:P:810:DT:C5'	2.42	0.50
3:A:376:THR:O	3:A:380:ILE:HG13	2.12	0.50
3:A:518:VAL:O	3:A:522:ILE:HG13	2.11	0.50
4:B:103:LYS:HE2	4:B:103:LYS:CA	2.36	0.50
4:B:244:ILE:HG12	4:B:244:ILE:O	2.11	0.50
4:B:63:ILE:HD12	4:B:407:GLN:HA	1.94	0.49
3:A:94:ILE:HG22	3:A:95:PRO:CD	2.41	0.49
3:A:394:GLN:C	3:A:396:GLU:N	2.69	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:406:TRP:C	4:B:331:LYS:HD3	2.37	0.49
3:A:444:GLY:HA3	3:A:455:ALA:CB	2.42	0.49
4:B:13:LYS:NZ	4:B:82:LYS:O	2.34	0.49
4:B:47:ILE:HA	4:B:145:GLN:O	2.12	0.49
4:B:85:GLN:HG2	4:B:86:ASP:N	2.26	0.49
4:B:426:TRP:N	4:B:426:TRP:HD1	2.05	0.49
3:A:425:LEU:HD13	3:A:509:GLN:HE22	1.76	0.49
3:A:451:LYS:CB	3:A:452:LEU:HD12	2.42	0.49
3:A:252:TRP:HB3	3:A:257:ILE:HD11	1.94	0.49
3:A:427:TYR:C	3:A:427:TYR:CD2	2.90	0.49
4:B:154:LYS:C	4:B:157:PRO:HD2	2.38	0.49
1:T:718:DA:H2''	1:T:719:DG:C5'	2.42	0.49
3:A:93:GLY:C	4:B:137:ASN:OD1	2.55	0.49
3:A:427:TYR:HE1	3:A:522:ILE:HG23	1.77	0.49
3:A:522:ILE:O	3:A:523:GLU:C	2.56	0.49
4:B:47:ILE:HG22	4:B:145:GLN:O	2.11	0.49
3:A:112:GLY:O	3:A:113:ASP:C	2.54	0.49
3:A:391:LEU:C	3:A:417:VAL:HG12	2.38	0.49
4:B:13:LYS:HA	4:B:85:GLN:NE2	2.27	0.49
4:B:292:VAL:HG12	4:B:294:PRO:HD3	1.95	0.49
4:B:332:GLN:NE2	4:B:424:LYS:HB3	2.25	0.49
4:B:334:GLN:O	4:B:334:GLN:CG	2.60	0.49
4:B:365:VAL:HG12	4:B:393:ILE:HD11	1.93	0.49
4:B:266:TRP:CD2	4:B:426:TRP:HH2	2.30	0.49
3:A:96:HIS:HE1	3:A:350:LYS:HG3	1.78	0.49
3:A:79:GLU:OE1	3:A:79:GLU:HA	2.12	0.49
4:B:100:LEU:HD13	4:B:381:VAL:HG13	1.94	0.49
2:P:814:DC:H2'	2:P:815:DG:C8	2.47	0.49
2:P:820:DC:H4'	3:A:266:TRP:CE2	2.48	0.49
3:A:517:LEU:CD2	3:A:521:ILE:HD11	2.43	0.48
4:B:34:LEU:HD11	4:B:60:VAL:CG2	2.43	0.48
4:B:42:GLU:C	4:B:44:GLU:H	2.21	0.48
4:B:111:VAL:HG21	4:B:164:MET:HE1	1.95	0.48
4:B:259:LYS:C	4:B:261:VAL:N	2.70	0.48
4:B:422:LEU:CA	4:B:425:LEU:HD13	2.42	0.48
3:A:354:TYR:HD2	3:A:371:ALA:CB	2.20	0.48
3:A:475:GLN:O	3:A:477:THR:N	2.47	0.48
4:B:13:LYS:NZ	4:B:16:MET:SD	2.80	0.48
4:B:239:TRP:HH2	4:B:353:LYS:O	1.97	0.48
4:B:410:TRP:O	4:B:411:ILE:HG13	2.13	0.48
3:A:273:GLY:N	3:A:338:THR:HG21	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:345:PRO:O	3:A:346:PHE:HB2	2.13	0.48
3:A:406:TRP:NE1	3:A:407:GLN:HG3	2.28	0.48
4:B:43:LYS:HG2	4:B:43:LYS:O	2.14	0.48
3:A:280:SER:OG	3:A:281:LYS:N	2.46	0.48
4:B:86:ASP:HB3	4:B:90:VAL:H	1.79	0.48
4:B:266:TRP:CB	4:B:426:TRP:CH2	2.97	0.48
4:B:376:THR:OG1	4:B:389:PHE:CZ	2.66	0.48
3:A:115:TYR:CE2	5:A:823:TNV:H8'1	2.49	0.48
3:A:406:TRP:O	4:B:331:LYS:HB3	2.14	0.48
3:A:432:GLU:CD	3:A:433:PRO:HD2	2.39	0.48
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.78	0.48
4:B:203:GLU:O	4:B:203:GLU:HG2	2.13	0.48
3:A:131:THR:OG1	3:A:143:ARG:HG2	2.14	0.48
4:B:109:LEU:CG	4:B:216:THR:HG21	2.40	0.48
4:B:60:VAL:O	4:B:60:VAL:HG23	2.11	0.48
3:A:127:TYR:C	3:A:129:ALA:H	2.22	0.47
3:A:225:PRO:HG3	3:A:227:PHE:CE1	2.48	0.47
3:A:261:VAL:HG12	3:A:265:ASN:ND2	2.29	0.47
3:A:333:GLY:C	3:A:334:GLN:HG2	2.39	0.47
3:A:465:LYS:O	3:A:466:VAL:HG13	2.14	0.47
4:B:34:LEU:HD11	4:B:60:VAL:HG21	1.96	0.47
2:P:803:DC:C2'	2:P:804:DA:OP1	2.61	0.47
3:A:28:GLU:CG	3:A:135:ILE:HG12	2.34	0.47
3:A:86:ASP:O	4:B:55:PRO:HB3	2.14	0.47
3:A:280:SER:C	3:A:282:LEU:N	2.71	0.47
3:A:417:VAL:O	3:A:417:VAL:CG1	2.61	0.47
3:A:435:VAL:O	3:A:436:GLY:C	2.56	0.47
3:A:469:LEU:CD2	3:A:480:GLN:HG2	2.44	0.47
4:B:135:ILE:HG13	4:B:135:ILE:O	2.14	0.47
4:B:406:TRP:CH2	4:B:412:PRO:HD2	2.49	0.47
3:A:65:ARG:HB2	3:A:68:SER:HB2	1.95	0.47
3:A:399:GLU:HA	3:A:402:TRP:NE1	2.29	0.47
3:A:444:GLY:HA3	3:A:455:ALA:HB2	1.95	0.47
4:B:86:ASP:O	4:B:87:PHE:C	2.57	0.47
3:A:90:VAL:O	3:A:90:VAL:HG22	2.14	0.47
3:A:368:LEU:HD21	3:A:391:LEU:HD22	1.96	0.47
3:A:396:GLU:C	3:A:398:TRP:N	2.72	0.47
4:B:307:ARG:O	4:B:311:LYS:NZ	2.47	0.47
4:B:388:LYS:O	4:B:388:LYS:HD3	2.15	0.47
4:B:100:LEU:O	4:B:101:LYS:C	2.56	0.47
4:B:237:ASP:C	4:B:239:TRP:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:282:LEU:HD22	4:B:295:LEU:HD23	1.94	0.47
3:A:276:VAL:CG2	3:A:353:LYS:NZ	2.78	0.47
3:A:435:VAL:HG22	4:B:290:THR:CG2	2.44	0.47
4:B:60:VAL:HG12	4:B:75:VAL:HG13	1.97	0.47
4:B:97:PRO:C	4:B:99:GLY:N	2.72	0.47
4:B:115:TYR:C	4:B:117:SER:H	2.23	0.47
4:B:125:ARG:C	4:B:127:TYR:H	2.23	0.47
4:B:126:LYS:HA	4:B:145:GLN:OE1	2.14	0.47
4:B:157:PRO:HB3	4:B:184:MET:O	2.14	0.47
4:B:234:LEU:HD11	4:B:377:THR:HG21	1.97	0.47
3:A:280:SER:O	3:A:281:LYS:C	2.57	0.47
4:B:169:GLU:HG2	4:B:170:PRO:HD3	1.94	0.47
4:B:175:ASN:HB3	4:B:178:ILE:HD12	1.97	0.47
4:B:401:TRP:O	4:B:404:GLU:HB2	2.15	0.47
3:A:194:GLU:HA	3:A:194:GLU:OE2	2.15	0.47
4:B:82:LYS:NZ	4:B:413:GLU:OE1	2.48	0.47
4:B:153:TRP:O	4:B:157:PRO:HD3	2.14	0.47
2:P:812:DT:H2'	2:P:813:DT:H6	1.78	0.47
3:A:247:PRO:HG2	3:A:260:LEU:HD11	1.97	0.47
3:A:429:LEU:HD11	3:A:506:ILE:HG22	1.96	0.47
3:A:441:TYR:HB2	3:A:458:VAL:CG2	2.45	0.47
4:B:245:VAL:HG22	4:B:246:LEU:N	2.30	0.47
2:P:808:DC:O2	2:P:808:DC:H2'	2.14	0.46
2:P:809:DC:H5'	3:A:475:GLN:CD	2.40	0.46
4:B:66:LYS:O	4:B:67:ASP:C	2.57	0.46
4:B:279:LEU:HD23	4:B:299:ALA:HB1	1.97	0.46
4:B:308:GLU:C	4:B:310:LEU:H	2.23	0.46
3:A:57:ASN:ND2	3:A:131:THR:OG1	2.48	0.46
3:A:363:ASN:HB2	3:A:511:ASP:OD2	2.16	0.46
3:A:407:GLN:HG2	4:B:392:PRO:O	2.15	0.46
4:B:116:PHE:CZ	4:B:151:GLN:HG3	2.51	0.46
3:A:35:VAL:HG22	3:A:132:ILE:HG21	1.97	0.46
3:A:398:TRP:C	3:A:400:THR:N	2.72	0.46
3:A:498:ASP:HA	3:A:536:VAL:O	2.15	0.46
4:B:91:GLN:O	4:B:91:GLN:HG2	2.16	0.46
3:A:420:PRO:HA	3:A:421:PRO:O	2.14	0.46
3:A:484:LEU:HD23	3:A:487:GLN:NE2	2.29	0.46
3:A:511:ASP:HA	3:A:522:ILE:HG21	1.96	0.46
4:B:64:LYS:NZ	4:B:69:THR:HG22	2.31	0.46
4:B:153:TRP:CE3	4:B:156:SER:N	2.83	0.46
3:A:438:GLU:CD	3:A:459:THR:HG21	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:472:THR:OG1	3:A:473:THR:N	2.48	0.46
4:B:235:HIS:N	4:B:236:PRO:HD3	2.30	0.46
1:T:704:DG:O6	3:A:30:LYS:NZ	2.48	0.46
3:A:65:ARG:CZ	3:A:70:LYS:HD2	2.45	0.46
3:A:92:LEU:N	3:A:92:LEU:HD23	2.30	0.46
3:A:253:THR:HG23	3:A:256:ASP:OD2	2.15	0.46
4:B:296:THR:O	4:B:300:GLU:HB2	2.15	0.46
4:B:297:GLU:HA	4:B:300:GLU:HB3	1.97	0.46
4:B:297:GLU:O	4:B:301:LEU:HB2	2.15	0.46
4:B:333:GLY:H	4:B:336:GLN:CB	2.29	0.46
4:B:388:LYS:HE2	4:B:415:GLU:OE1	2.15	0.46
3:A:420:PRO:CA	3:A:421:PRO:C	2.84	0.46
3:A:427:TYR:HE1	3:A:522:ILE:CG2	2.29	0.46
4:B:86:ASP:HB3	4:B:90:VAL:HG23	1.97	0.46
4:B:125:ARG:HE	4:B:147:ASN:HA	1.81	0.46
4:B:278:GLN:O	4:B:299:ALA:HB2	2.14	0.46
4:B:394:GLN:O	4:B:395:LYS:C	2.58	0.46
3:A:34:LEU:HB3	3:A:132:ILE:HD13	1.98	0.46
3:A:409:THR:O	4:B:364:ASP:OD2	2.33	0.46
4:B:318:TYR:CD1	4:B:318:TYR:N	2.84	0.46
4:B:421:PRO:HA	4:B:423:VAL:HG22	1.98	0.46
2:P:805:DG:C5	2:P:806:DT:C5	3.04	0.46
3:A:194:GLU:O	3:A:195:ILE:C	2.59	0.46
3:A:222:GLN:C	3:A:224:GLU:H	2.23	0.46
3:A:306:ASN:O	3:A:308:GLU:N	2.49	0.46
4:B:143:ARG:O	4:B:144:TYR:CG	2.69	0.46
4:B:53:GLU:OE2	4:B:53:GLU:N	2.48	0.46
3:A:391:LEU:HA	3:A:392:PRO:HD3	1.59	0.45
3:A:426:TRP:O	3:A:427:TYR:HB3	2.15	0.45
3:A:452:LEU:HD12	3:A:452:LEU:N	2.31	0.45
3:A:476:LYS:O	3:A:480:GLN:HB2	2.15	0.45
4:B:62:ALA:C	4:B:63:ILE:HG23	2.41	0.45
4:B:153:TRP:HE3	4:B:156:SER:HB2	1.81	0.45
4:B:240:THR:CG2	4:B:241:VAL:N	2.79	0.45
4:B:282:LEU:H	4:B:282:LEU:CD1	2.26	0.45
3:A:354:TYR:HE1	3:A:356:ARG:HB3	1.81	0.45
3:A:446:ALA:HB2	3:A:453:GLY:HA3	1.98	0.45
4:B:109:LEU:CD1	4:B:216:THR:HG21	2.47	0.45
1:T:707:DG:O3'	3:A:89:GLU:HG2	2.17	0.45
4:B:362:THR:HB	4:B:366:LYS:HD3	1.97	0.45
3:A:63:ILE:CG2	3:A:64:LYS:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:329:ILE:HG22	4:B:392:PRO:HD3	1.97	0.45
3:A:358:ARG:NH1	4:B:396:GLU:HG2	2.31	0.45
3:A:396:GLU:O	3:A:398:TRP:N	2.50	0.45
3:A:489:SER:HB2	3:A:493:VAL:HG22	1.99	0.45
4:B:234:LEU:C	4:B:235:HIS:CG	2.94	0.45
3:A:244:ILE:HD12	3:A:266:TRP:CD1	2.51	0.45
4:B:275:LYS:HB2	4:B:306:ASN:HD21	1.81	0.45
4:B:350:LYS:HB3	4:B:383:TRP:HH2	1.82	0.45
4:B:421:PRO:CB	4:B:424:LYS:HG3	2.47	0.45
3:A:81:ASN:OD1	3:A:154:LYS:HB2	2.17	0.45
3:A:282:LEU:CD1	3:A:296:THR:HG23	2.46	0.45
3:A:519:ASN:HA	3:A:522:ILE:HD12	1.98	0.45
4:B:5:ILE:HG22	4:B:6:GLU:H	1.81	0.45
4:B:275:LYS:N	4:B:306:ASN:OD1	2.49	0.45
1:T:719:DG:C6	1:T:720:DG:C6	3.05	0.45
3:A:438:GLU:OE2	3:A:459:THR:HG21	2.17	0.45
3:A:442:VAL:CG2	3:A:481:ALA:HB1	2.47	0.45
4:B:211:ARG:HA	4:B:211:ARG:HD3	1.71	0.45
4:B:323:LYS:HD2	4:B:323:LYS:HA	1.79	0.45
4:B:81:ASN:CA	4:B:84:THR:HG22	2.42	0.45
4:B:333:GLY:H	4:B:336:GLN:HB3	1.82	0.45
1:T:713:DC:H2'	1:T:714:DG:C8	2.52	0.45
3:A:249:LYS:HE3	3:A:256:ASP:OD1	2.18	0.45
3:A:394:GLN:HA	3:A:394:GLN:OE1	2.16	0.45
4:B:14:PRO:HD3	4:B:85:GLN:NE2	2.32	0.45
4:B:266:TRP:C	4:B:268:SER:N	2.71	0.45
1:T:716:DA:C2'	1:T:717:DC:O4'	2.65	0.44
3:A:13:LYS:O	3:A:14:PRO:C	2.60	0.44
3:A:371:ALA:O	3:A:372:VAL:C	2.61	0.44
4:B:330:GLN:OE1	4:B:340:GLN:NE2	2.49	0.44
3:A:406:TRP:HB2	4:B:424:LYS:NZ	2.32	0.44
3:A:522:ILE:O	3:A:525:LEU:N	2.50	0.44
4:B:13:LYS:HB2	4:B:13:LYS:HE3	1.79	0.44
3:A:398:TRP:C	3:A:400:THR:H	2.25	0.44
3:A:417:VAL:HG13	3:A:419:THR:HG22	2.00	0.44
3:A:431:LYS:HA	3:A:431:LYS:HD3	1.77	0.44
4:B:70:LYS:HD3	4:B:70:LYS:HA	1.73	0.44
4:B:77:PHE:O	4:B:78:ARG:C	2.61	0.44
4:B:149:LEU:HD23	4:B:149:LEU:HA	1.81	0.44
4:B:361:HIS:H	4:B:361:HIS:HD2	1.62	0.44
1:T:706:DC:H2'	1:T:707:DG:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:451:LYS:HB2	3:A:452:LEU:HD12	2.00	0.44
3:A:459:THR:HG21	3:A:463:ARG:HB3	1.98	0.44
4:B:66:LYS:O	4:B:66:LYS:CG	2.66	0.44
4:B:108:VAL:HG13	4:B:188:TYR:CE2	2.52	0.44
4:B:367:GLN:O	4:B:368:LEU:C	2.60	0.44
1:T:705:DT:C2	3:A:74:LEU:HD13	2.52	0.44
3:A:255:ASN:OD1	3:A:255:ASN:C	2.59	0.44
3:A:498:ASP:HB2	3:A:538:ALA:HB2	1.99	0.44
4:B:80:LEU:HD23	4:B:153:TRP:CD1	2.52	0.44
2:P:805:DG:C2	2:P:806:DT:C2	3.06	0.44
3:A:61:PHE:CD1	3:A:61:PHE:N	2.86	0.44
3:A:88:TRP:CB	4:B:143:ARG:NH1	2.78	0.44
3:A:224:GLU:N	3:A:225:PRO:CD	2.81	0.44
3:A:481:ALA:C	3:A:483:TYR:N	2.74	0.44
3:A:257:ILE:HB	3:A:283:LEU:HD21	1.99	0.44
4:B:3:SER:O	4:B:5:ILE:HG13	2.18	0.44
4:B:91:GLN:O	4:B:92:LEU:HD23	2.17	0.44
4:B:178:ILE:HG23	4:B:190:GLY:O	2.18	0.44
3:A:90:VAL:HG22	4:B:140:PRO:HB2	1.99	0.44
3:A:199:ARG:O	3:A:202:ILE:HG22	2.18	0.44
3:A:221:HIS:CE1	3:A:228:LEU:HB2	2.47	0.44
3:A:386:THR:HA	3:A:387:PRO:HD3	1.78	0.44
4:B:50:ILE:HD13	4:B:145:GLN:HG3	2.00	0.44
4:B:209:LEU:HB3	4:B:214:LEU:HD12	2.00	0.44
1:T:708:DG:H2'	1:T:709:DC:H6	1.82	0.44
3:A:282:LEU:CD2	3:A:295:LEU:HD23	2.46	0.44
3:A:369:THR:HG23	3:A:411:ILE:HD11	1.98	0.44
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.53	0.43
3:A:550:LYS:C	3:A:552:VAL:N	2.74	0.43
4:B:255:ASN:ND2	4:B:259:LYS:HE2	2.32	0.43
1:T:718:DA:H2''	1:T:719:DG:O5'	2.17	0.43
3:A:320:ASP:HA	3:A:321:PRO:HD2	1.82	0.43
3:A:546:GLU:O	3:A:550:LYS:HG3	2.18	0.43
4:B:66:LYS:HG3	4:B:68:SER:HB3	2.00	0.43
4:B:269:GLN:HE21	4:B:269:GLN:HB2	1.58	0.43
4:B:270:ILE:HD12	4:B:314:VAL:HG21	2.00	0.43
1:T:707:DG:H2'	1:T:708:DG:C8	2.53	0.43
3:A:21:VAL:CG2	3:A:22:LYS:N	2.81	0.43
3:A:242:GLN:O	3:A:243:PRO:C	2.62	0.43
3:A:288:ALA:HB3	3:A:291:GLU:HB2	1.98	0.43
3:A:435:VAL:HG12	3:A:436:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:30:LYS:O	4:B:34:LEU:HB2	2.18	0.43
4:B:250:ASP:C	4:B:251:SER:HG	2.27	0.43
4:B:293:ILE:CG1	4:B:293:ILE:O	2.65	0.43
3:A:435:VAL:HG13	4:B:290:THR:HG21	2.00	0.43
4:B:60:VAL:HG11	4:B:130:PHE:CD2	2.53	0.43
4:B:183:TYR:CD2	4:B:380:ILE:HD13	2.52	0.43
4:B:410:TRP:C	4:B:411:ILE:HG13	2.42	0.43
4:B:421:PRO:HB2	4:B:422:LEU:H	1.63	0.43
3:A:281:LYS:C	3:A:283:LEU:H	2.26	0.43
3:A:406:TRP:O	4:B:331:LYS:HD3	2.19	0.43
4:B:271:TYR:CD2	4:B:309:ILE:HG22	2.53	0.43
3:A:255:ASN:OD1	3:A:256:ASP:N	2.51	0.43
4:B:42:GLU:OE2	4:B:49:LYS:HG3	2.19	0.43
4:B:345:PRO:O	4:B:346:PHE:CB	2.67	0.43
4:B:418:ASN:O	4:B:418:ASN:CG	2.62	0.43
4:B:424:LYS:O	4:B:428:GLN:HB2	2.18	0.43
4:B:53:GLU:O	4:B:55:PRO:HD3	2.18	0.43
3:A:8:VAL:HA	3:A:9:PRO:HD3	1.80	0.43
3:A:34:LEU:HB3	3:A:132:ILE:CD1	2.49	0.43
3:A:67:ASP:CG	3:A:67:ASP:O	2.61	0.43
3:A:242:GLN:HB3	3:A:243:PRO:HD2	2.00	0.43
3:A:300:GLU:OE1	3:A:300:GLU:HA	2.18	0.43
1:T:720:DG:H2'	1:T:721:DG:H8	1.75	0.43
3:A:280:SER:O	3:A:282:LEU:N	2.52	0.43
3:A:306:ASN:C	3:A:308:GLU:N	2.76	0.43
3:A:319:TYR:HE1	3:A:325:LEU:HD13	1.84	0.43
4:B:27:THR:O	4:B:28:GLU:C	2.61	0.43
4:B:106:VAL:HG12	4:B:107:THR:N	2.34	0.43
4:B:114:ALA:CB	4:B:214:LEU:CD2	2.96	0.43
3:A:72:ARG:HG2	3:A:74:LEU:HD21	2.01	0.43
3:A:93:GLY:CA	4:B:137:ASN:OD1	2.67	0.43
3:A:366:LYS:HE2	3:A:401:TRP:HH2	1.83	0.43
4:B:277:ARG:HG2	4:B:277:ARG:HH11	1.83	0.43
4:B:319:TYR:CD1	4:B:383:TRP:CD1	3.07	0.43
3:A:279:LEU:N	3:A:302:GLU:OE2	2.51	0.42
3:A:454:LYS:HA	3:A:469:LEU:HG	2.00	0.42
4:B:86:ASP:C	4:B:88:TRP:N	2.76	0.42
4:B:314:VAL:HG22	4:B:315:HIS:H	1.83	0.42
3:A:63:ILE:HG22	3:A:64:LYS:O	2.19	0.42
3:A:416:PHE:HZ	3:A:422:LEU:HD11	1.84	0.42
4:B:305:GLU:C	4:B:307:ARG:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:714:DG:OP1	3:A:284:ARG:HB3	2.20	0.42
3:A:441:TYR:CE2	3:A:544:GLY:HA3	2.53	0.42
3:A:451:LYS:HB3	3:A:452:LEU:HD12	2.02	0.42
4:B:75:VAL:HB	4:B:77:PHE:CE2	2.54	0.42
1:T:703:DG:C2'	1:T:704:DG:O5'	2.67	0.42
1:T:708:DG:H4'	3:A:91:GLN:O	2.19	0.42
1:T:719:DG:C2	1:T:720:DG:C4	3.07	0.42
2:P:809:DC:H5'	3:A:475:GLN:NE2	2.34	0.42
3:A:77:PHE:O	3:A:81:ASN:ND2	2.52	0.42
3:A:288:ALA:C	3:A:290:THR:N	2.73	0.42
3:A:478:GLU:HG2	3:A:499:SER:CB	2.46	0.42
4:B:361:HIS:CD2	4:B:361:HIS:N	2.82	0.42
3:A:416:PHE:CE2	3:A:418:ASN:HB2	2.54	0.42
3:A:467:VAL:HG13	3:A:468:PRO:HD2	2.02	0.42
4:B:164:MET:O	4:B:165:THR:C	2.61	0.42
4:B:279:LEU:CD2	4:B:295:LEU:HD22	2.50	0.42
4:B:393:ILE:CG2	4:B:398:TRP:HB2	2.50	0.42
1:T:709:DC:H2'	1:T:710:DG:C8	2.55	0.42
3:A:164:MET:HG3	3:A:182:GLN:NE2	2.34	0.42
4:B:210:LEU:HA	4:B:214:LEU:O	2.19	0.42
4:B:320:ASP:OD1	4:B:322:SER:HB3	2.19	0.42
4:B:366:LYS:O	4:B:370:GLU:HG3	2.19	0.42
3:A:21:VAL:HG22	3:A:22:LYS:N	2.35	0.42
4:B:257:ILE:C	4:B:259:LYS:N	2.77	0.42
4:B:264:LEU:HA	4:B:267:ALA:HB3	2.02	0.42
3:A:28:GLU:O	3:A:32:LYS:HG3	2.20	0.42
3:A:235:HIS:HB2	3:A:238:LYS:O	2.20	0.42
3:A:391:LEU:HB2	3:A:414:TRP:CE3	2.54	0.42
3:A:498:ASP:CG	3:A:538:ALA:HB2	2.45	0.42
4:B:354:TYR:HD2	4:B:371:ALA:HB2	1.85	0.42
1:T:708:DG:H5'	3:A:89:GLU:CG	2.49	0.42
3:A:64:LYS:HD3	3:A:71:TRP:CZ2	2.54	0.42
4:B:78:ARG:HD3	4:B:411:ILE:O	2.19	0.42
4:B:271:TYR:C	4:B:273:GLY:N	2.78	0.42
3:A:22:LYS:HG2	3:A:23:GLN:N	2.34	0.42
3:A:490:GLY:O	3:A:528:LYS:HD2	2.19	0.42
4:B:10:VAL:HG13	4:B:87:PHE:CD1	2.55	0.42
3:A:91:GLN:HB2	3:A:161:GLN:NE2	2.34	0.41
3:A:444:GLY:CA	3:A:552:VAL:HG11	2.45	0.41
4:B:326:ILE:CG2	4:B:327:ALA:H	2.32	0.41
3:A:363:ASN:OD1	3:A:365:VAL:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:446:ALA:HB2	3:A:472:THR:HG23	2.02	0.41
4:B:26:LEU:HD12	4:B:31:ILE:HG12	2.02	0.41
4:B:266:TRP:O	4:B:269:GLN:NE2	2.53	0.41
3:A:350:LYS:HG2	3:A:351:THR:N	2.34	0.41
3:A:550:LYS:O	3:A:552:VAL:N	2.54	0.41
2:P:813:DT:H2'	2:P:814:DC:C6	2.55	0.41
3:A:393:ILE:HG23	3:A:393:ILE:O	2.19	0.41
4:B:170:PRO:HB2	4:B:208:HIS:CE1	2.56	0.41
4:B:202:ILE:O	4:B:206:ARG:HG3	2.21	0.41
4:B:330:GLN:NE2	4:B:340:GLN:HE22	2.19	0.41
1:T:707:DG:H2''	1:T:708:DG:H5'	2.03	0.41
3:A:23:GLN:CD	3:A:59:PRO:HA	2.45	0.41
3:A:87:PHE:N	3:A:87:PHE:CD1	2.89	0.41
3:A:411:ILE:HA	3:A:412:PRO:HD3	1.89	0.41
3:A:434:ILE:CD1	3:A:530:LYS:HB3	2.36	0.41
3:A:458:VAL:HA	3:A:463:ARG:O	2.21	0.41
3:A:50:ILE:CG2	3:A:145:GLN:HG2	2.50	0.41
3:A:452:LEU:HB3	3:A:453:GLY:H	1.66	0.41
4:B:391:LEU:HA	4:B:392:PRO:HD3	1.95	0.41
3:A:446:ALA:CA	3:A:453:GLY:HA3	2.50	0.41
4:B:50:ILE:O	4:B:143:ARG:HB2	2.20	0.41
4:B:153:TRP:HB3	4:B:156:SER:HB2	2.01	0.41
4:B:195:ILE:HD11	4:B:199:ARG:NH2	2.36	0.41
4:B:233:GLU:CD	4:B:233:GLU:H	2.26	0.41
4:B:240:THR:CG2	4:B:241:VAL:H	2.34	0.41
2:P:816:DG:H2'	2:P:817:MRG:C8	2.50	0.41
3:A:146:TYR:CG	3:A:150:PRO:HB3	2.56	0.41
3:A:247:PRO:CG	3:A:260:LEU:CD1	2.99	0.41
4:B:206:ARG:HB3	4:B:206:ARG:CZ	2.51	0.41
4:B:365:VAL:HG23	4:B:366:LYS:N	2.35	0.41
2:P:805:DG:C4	2:P:806:DT:C6	3.09	0.41
3:A:18:GLY:HA3	3:A:56:TYR:CE1	2.55	0.41
3:A:42:GLU:HG3	3:A:144:TYR:HE2	1.86	0.41
3:A:68:SER:HB3	3:A:70:LYS:HB3	2.02	0.41
3:A:94:ILE:CG2	3:A:95:PRO:CD	2.96	0.41
3:A:107:THR:HB	3:A:202:ILE:HD11	2.03	0.41
3:A:375:ILE:O	3:A:379:SER:HB3	2.21	0.41
3:A:395:LYS:HD2	3:A:395:LYS:HA	1.89	0.41
3:A:417:VAL:HG22	3:A:419:THR:HG22	2.02	0.41
3:A:492:GLU:HG2	3:A:530:LYS:HB2	2.03	0.41
4:B:111:VAL:C	4:B:113:ASP:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:206:ARG:HH11	4:B:206:ARG:CB	2.33	0.41
4:B:254:VAL:O	4:B:258:GLN:HG3	2.20	0.41
4:B:259:LYS:O	4:B:260:LEU:C	2.63	0.41
4:B:395:LYS:HE2	4:B:399:GLU:OE1	2.21	0.41
3:A:58:THR:CG2	3:A:59:PRO:HD2	2.50	0.41
3:A:286:THR:O	3:A:287:LYS:HG2	2.21	0.41
3:A:491:LEU:HD22	3:A:529:GLU:HG2	2.03	0.41
4:B:32:LYS:O	4:B:35:VAL:HG12	2.20	0.41
4:B:118:VAL:O	4:B:118:VAL:HG12	2.19	0.41
4:B:241:VAL:HA	4:B:351:THR:O	2.21	0.41
4:B:422:LEU:HD12	4:B:425:LEU:CD1	2.51	0.41
1:T:715:DA:C6	1:T:716:DA:C6	3.10	0.40
3:A:486:LEU:HD13	3:A:524:GLN:HB2	2.03	0.40
4:B:164:MET:O	4:B:167:ILE:N	2.54	0.40
4:B:365:VAL:CG1	4:B:393:ILE:HD11	2.51	0.40
1:T:715:DA:H2''	1:T:716:DA:C5'	2.51	0.40
2:P:808:DC:H2''	3:A:475:GLN:CD	2.44	0.40
3:A:151:GLN:HE21	3:A:151:GLN:HB2	1.74	0.40
4:B:178:ILE:HD11	4:B:201:LYS:HZ3	1.82	0.40
3:A:540:LYS:O	3:A:541:GLY:C	2.64	0.40
4:B:42:GLU:C	4:B:44:GLU:N	2.79	0.40
4:B:82:LYS:HZ3	4:B:413:GLU:CD	2.28	0.40
4:B:125:ARG:C	4:B:127:TYR:N	2.79	0.40
4:B:210:LEU:C	4:B:212:TRP:H	2.29	0.40
4:B:268:SER:O	4:B:271:TYR:O	2.39	0.40
4:B:278:GLN:HB3	4:B:299:ALA:HA	2.03	0.40
4:B:279:LEU:CD2	4:B:299:ALA:HB1	2.51	0.40
1:T:705:DT:H2'	1:T:706:DC:H6	1.87	0.40
3:A:306:ASN:O	3:A:309:ILE:N	2.55	0.40
3:A:319:TYR:CE1	3:A:325:LEU:HD13	2.56	0.40
3:A:410:TRP:CG	3:A:411:ILE:N	2.89	0.40
3:A:482:ILE:HG23	3:A:495:ILE:HG21	2.03	0.40
3:A:484:LEU:CA	3:A:487:GLN:HE21	2.15	0.40
3:A:489:SER:OG	3:A:493:VAL:HG21	2.22	0.40
4:B:115:TYR:HB3	4:B:149:LEU:HB2	2.04	0.40
2:P:819:DG:H2'	2:P:820:DC:H6	1.86	0.40
3:A:21:VAL:HG13	3:A:59:PRO:CD	2.50	0.40
3:A:158:ALA:HB1	4:B:52:PRO:HB3	2.03	0.40
3:A:443:ASP:CG	3:A:444:GLY:N	2.79	0.40
3:A:537:PRO:HG2	3:A:542:ILE:HD11	2.03	0.40
4:B:108:VAL:HG13	4:B:188:TYR:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:193:LEU:HB2	4:B:198:HIS:HB2	2.04	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	
3	A	552/558 (99%)	449 (81%)	92 (17%)	11 (2%)	6	28
4	B	409/437 (94%)	310 (76%)	81 (20%)	18 (4%)	2	12
All	All	961/995 (97%)	759 (79%)	173 (18%)	29 (3%)	3	19

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	98	ALA
3	A	485	ALA
3	A	541	GLY
4	B	86	ASP
4	B	112	GLY
4	B	282	LEU
3	A	307	ARG
3	A	476	LYS
4	B	113	ASP
4	B	214	LEU
4	B	260	LEU
4	B	294	PRO
4	B	316	GLY
4	B	421	PRO
4	B	85	GLN
4	B	119	PRO
4	B	126	LYS

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Mol	Chain	Res	Type
3	A	116	PHE
3	A	551	LEU
4	B	314	VAL
4	B	379	SER
3	A	224	GLU
3	A	509	GLN
4	B	387	PRO
3	A	14	PRO
4	B	4	PRO
3	A	420	PRO
4	B	13	LYS
3	A	433	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	495/498 (99%)	463 (94%)	32 (6%)	15	47
4	B	375/397 (94%)	339 (90%)	36 (10%)	8	31
All	All	870/895 (97%)	802 (92%)	68 (8%)	11	39

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	14	PRO
3	A	21	VAL
3	A	25	PRO
3	A	27	THR
3	A	53	GLU
3	A	79	GLU
3	A	86	ASP
3	A	89	GLU
3	A	132	ILE
3	A	151	GLN
3	A	156	SER

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Mol	Chain	Res	Type
3	A	165	THR
3	A	173	LYS
3	A	188	TYR
3	A	202	ILE
3	A	224	GLU
3	A	226	PRO
3	A	236	PRO
3	A	240	THR
3	A	249	LYS
3	A	250	ASP
3	A	260	LEU
3	A	270	ILE
3	A	330	GLN
3	A	340	GLN
3	A	369	THR
3	A	373	GLN
3	A	393	ILE
3	A	403	THR
3	A	426	TRP
3	A	514	GLU
3	A	548	VAL
4	B	16	MET
4	B	17	ASP
4	B	24	TRP
4	B	28	GLU
4	B	29	GLU
4	B	31	ILE
4	B	34	LEU
4	B	40	GLU
4	B	69	THR
4	B	119	PRO
4	B	137	ASN
4	B	139	THR
4	B	145	GLN
4	B	174	GLN
4	B	189	VAL
4	B	210	LEU
4	B	233	GLU
4	B	235	HIS
4	B	251	SER
4	B	255	ASN
4	B	269	GLN

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Mol	Chain	Res	Type
4	B	274	ILE
4	B	290	THR
4	B	293	ILE
4	B	295	LEU
4	B	303	LEU
4	B	318	TYR
4	B	329	ILE
4	B	340	GLN
4	B	344	GLU
4	B	361	HIS
4	B	368	LEU
4	B	375	ILE
4	B	392	PRO
4	B	396	GLU
4	B	426	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	57	ASN
3	A	137	ASN
3	A	161	GLN
3	A	221	HIS
3	A	428	GLN
3	A	447	ASN
3	A	464	GLN
3	A	471	ASN
3	A	487	GLN
3	A	494	ASN
3	A	509	GLN
3	A	520	GLN
3	A	545	ASN
4	B	85	GLN
4	B	91	GLN
4	B	161	GLN
4	B	242	GLN
4	B	269	GLN
4	B	330	GLN
4	B	334	GLN
4	B	340	GLN
4	B	348	ASN
4	B	361	HIS

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Mol	Chain	Res	Type
4	B	363	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
2	DDG	P	822	1,2	20,23,24	0.42	0	27,33,36	0.34	0
2	MRG	P	817	1,3,2	25,28,29	1.39	1 (4%)	32,39,42	1.71	1 (3%)

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	DDG	P	822	1,2	-	0/7/18/19	0/3/3/3
2	MRG	P	817	1,3,2	-	3/12/26/27	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	817	MRG	C21-N2	-6.66	1.31	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	817	MRG	C21-N2-C2	-9.36	105.78	123.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	817	MRG	N1-C2-N2-C21
2	P	817	MRG	C21-C22-C23-S24
2	P	817	MRG	N3-C2-N2-C21

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	822	DDG	2	0
2	P	817	MRG	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are 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	SO4	A	560	-	4,4,4	0.62	0	6,6,6	0.37	0
7	SO4	A	559	-	4,4,4	0.70	0	6,6,6	0.20	0
5	TNV	A	823	6	26,28,28	1.40	4 (15%)	36,43,43	1.23	5 (13%)

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
5	TNV	A	823	6	-	2/19/22/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	823	TNV	PB-O3A	-3.56	1.55	1.59
5	A	823	TNV	PA-O3A	-3.40	1.54	1.58
5	A	823	TNV	PA-O1A	2.04	1.56	1.51
5	A	823	TNV	PB-O3B	-2.03	1.57	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	823	TNV	PA-C9'-O9'	-3.70	102.37	109.06
5	A	823	TNV	O3G-PG-O3B	2.82	114.10	104.64
5	A	823	TNV	C4-N9-C8	2.23	107.35	105.75
5	A	823	TNV	O3A-PA-C9'	2.22	113.76	104.01
5	A	823	TNV	N9-C8-N7	-2.00	112.31	114.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	823	TNV	C6'-C7'-O9'-C9'
5	A	823	TNV	PA-O3A-PB-O2B

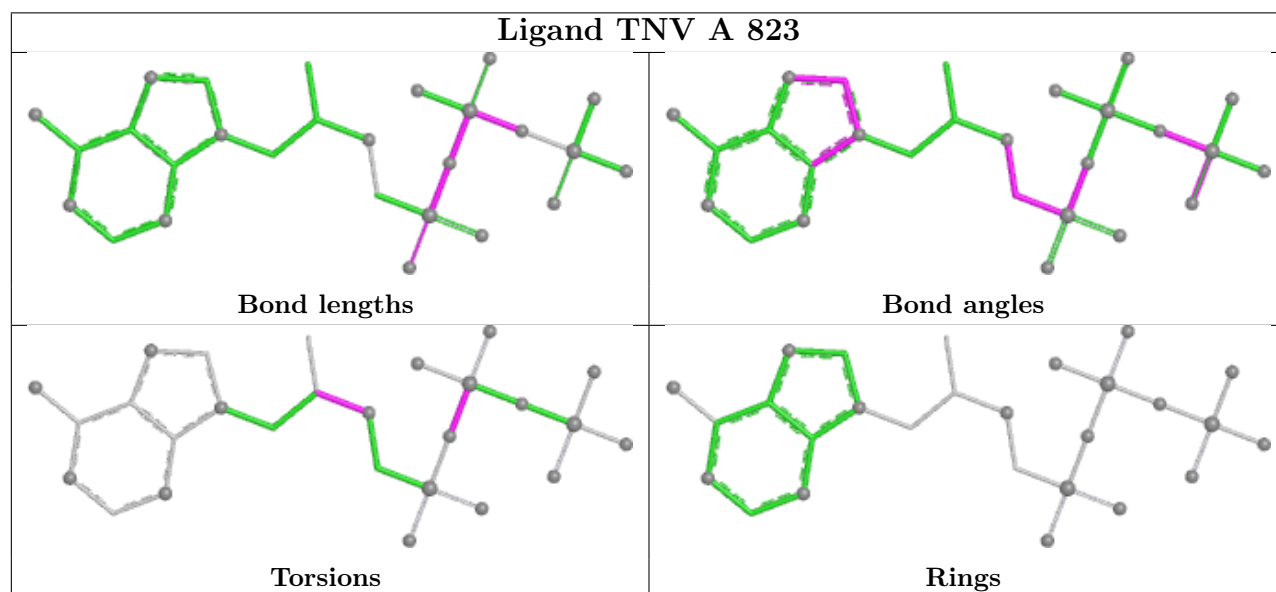
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	823	TNV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	T	24/27 (88%)	0.50	1 (4%)	40	22	40, 111, 138, 143	0
2	P	18/21 (85%)	0.56	1 (5%)	30	15	46, 105, 145, 150	0
3	A	554/558 (99%)	0.11	17 (3%)	51	30	24, 70, 131, 149	0
4	B	413/437 (94%)	0.71	50 (12%)	8	5	41, 105, 147, 150	0
All	All	1009/1043 (96%)	0.38	69 (6%)	23	12	24, 85, 141, 150	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	5	ILE	6.6
4	B	422	LEU	4.5
4	B	425	LEU	4.4
4	B	94	ILE	4.3
4	B	426	TRP	4.2
3	A	554	ALA	4.2
4	B	95	PRO	4.1
3	A	122	GLU	3.7
4	B	88	TRP	3.6
4	B	97	PRO	3.5
4	B	276	VAL	3.5
4	B	286	THR	3.4
4	B	303	LEU	3.4
3	A	428	GLN	3.4
4	B	90	VAL	3.3
4	B	236	PRO	3.2
4	B	318	TYR	3.2
4	B	316	GLY	3.1
4	B	362	THR	3.1
4	B	92	LEU	3.0
4	B	214	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
4	B	294	PRO	2.8
4	B	423	VAL	2.8
4	B	85	GLN	2.8
4	B	420	PRO	2.8
3	A	538	ALA	2.7
4	B	417	VAL	2.7
3	A	474	ASN	2.7
4	B	336	GLN	2.6
4	B	89	GLU	2.6
3	A	493	VAL	2.6
4	B	360	ALA	2.6
3	A	438	GLU	2.6
4	B	292	VAL	2.6
4	B	428	GLN	2.5
3	A	476	LYS	2.5
4	B	3	SER	2.4
4	B	239	TRP	2.4
4	B	357	MET	2.4
4	B	418	ASN	2.4
4	B	213	GLY	2.4
4	B	67	ASP	2.4
2	P	803	DC	2.4
3	A	452	LEU	2.4
3	A	491	LEU	2.4
4	B	314	VAL	2.4
3	A	356	ARG	2.3
4	B	193	LEU	2.3
3	A	135	ILE	2.3
3	A	298	GLU	2.3
3	A	537	PRO	2.3
4	B	172	LYS	2.2
4	B	358	ARG	2.2
3	A	478	GLU	2.2
4	B	371	ALA	2.2
4	B	275	LYS	2.2
1	T	725	DG	2.2
4	B	242	GLN	2.2
4	B	65	LYS	2.2
3	A	512	LYS	2.1
4	B	424	LYS	2.1
4	B	7	THR	2.1
4	B	339	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	266	TRP	2.1
4	B	96	HIS	2.1
4	B	361	HIS	2.1
4	B	217	PRO	2.1
4	B	241	VAL	2.0
3	A	289	LEU	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	MRG	P	817	26/27	0.88	0.14	57,68,85,93	0
2	DDG	P	822	21/22	0.98	0.07	38,50,62,72	0

6.3 Carbohydrates [i](#)

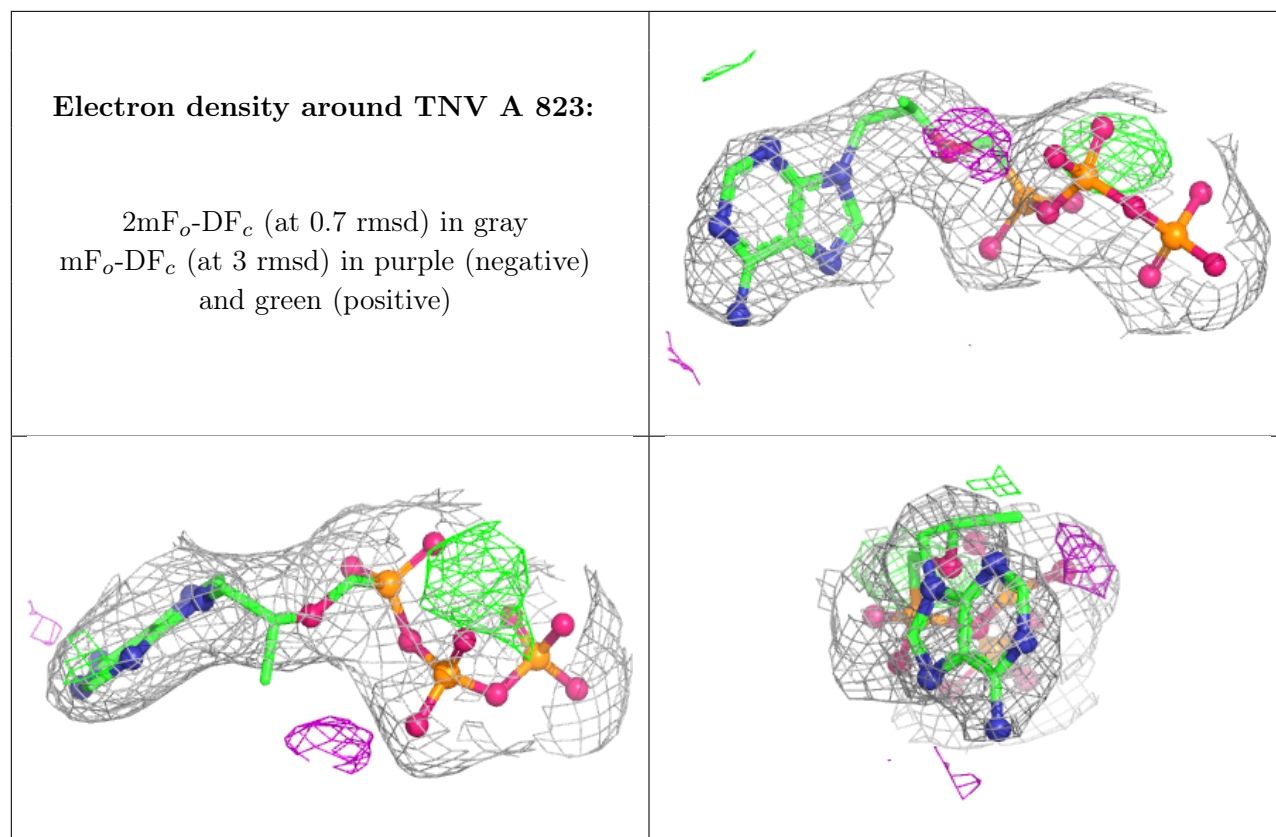
There are no oligosaccharides in this entry.

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	SO4	A	559	5/5	0.64	0.15	131,132,136,137	0
7	SO4	A	560	5/5	0.93	0.20	113,115,119,119	0
6	MG	A	601	1/1	0.96	0.05	75,75,75,75	0
5	TNV	A	823	27/27	0.98	0.08	40,58,66,75	0
6	MG	A	600	1/1	1.00	0.11	33,33,33,33	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.