



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:01 AM UTC

PDB ID : 1P7H / pdb_00001p7h
Title : Structure of NFAT1 bound as a dimer to the HIV-1 LTR kB element
Authors : Giffin, M.J.; Stroud, J.C.; Bates, D.L.; von Koenig, K.D.; Hardin, J.; Chen, L.
Deposited on : 2003-05-01
Resolution : 2.60 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
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

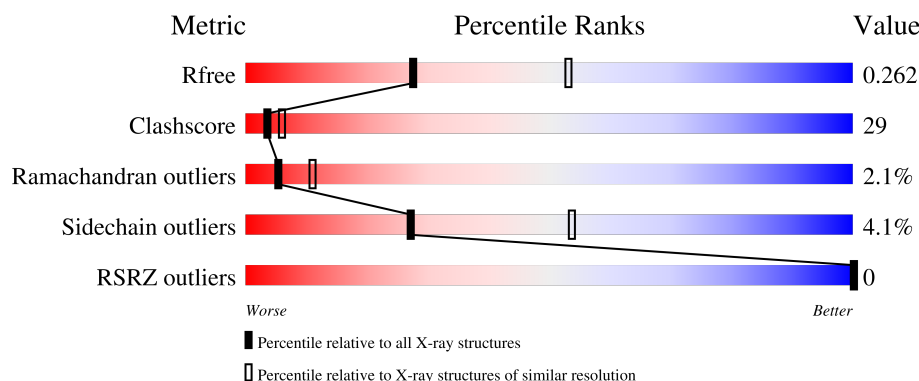
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	15	40% 60%
1	C	15	13% 80% 7%
2	B	15	53% 47%
2	D	15	53% 47%
3	L	286	55% 40% 5%

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Mol	Chain	Length	Quality of chain
3	M	286	 56% 41% •
3	N	286	 54% 41% 5% •
3	O	286	 54% 43% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10395 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(*AP*AP*TP*GP*GP*GP*GP*AP*CP*TP*TP*TP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			306	147	57	88	14			
1	C	15	Total	C	N	O	P	0	0	0
			306	147	57	88	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			303	146	55	88	14			
2	D	15	Total	C	N	O	P	0	0	0
			303	146	55	88	14			

- Molecule 3 is a protein called Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	286	Total	C	N	O	S	0	0	0
			2247	1410	410	418	9			
3	M	286	Total	C	N	O	S	0	0	0
			2247	1410	410	418	9			
3	N	286	Total	C	N	O	S	0	0	0
			2247	1410	410	418	9			
3	O	286	Total	C	N	O	S	0	0	0
			2247	1410	410	418	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	394	SER	LEU	conflict	UNP Q13469
L	395	VAL	PRO	conflict	UNP Q13469

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Chain	Residue	Modelled	Actual	Comment	Reference
M	394	SER	LEU	conflict	UNP Q13469
M	395	VAL	PRO	conflict	UNP Q13469
N	394	SER	LEU	conflict	UNP Q13469
N	395	VAL	PRO	conflict	UNP Q13469
O	394	SER	LEU	conflict	UNP Q13469
O	395	VAL	PRO	conflict	UNP Q13469

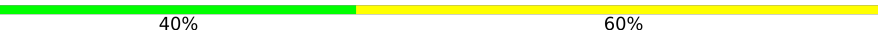
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	3	Total O 3 3	0	0
4	C	11	Total O 11 11	0	0
4	D	7	Total O 7 7	0	0
4	L	41	Total O 41 41	0	0
4	M	40	Total O 40 40	0	0
4	N	41	Total O 41 41	0	0
4	O	40	Total O 40 40	0	0

3 Residue-property plots

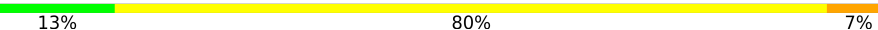
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-D(*AP*AP*TP*GP*GP*GP*GP*AP*CP*TP*TP*TP*CP*CP*A)-3'

Chain A: 



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

Chain C: 



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

Chain B: 



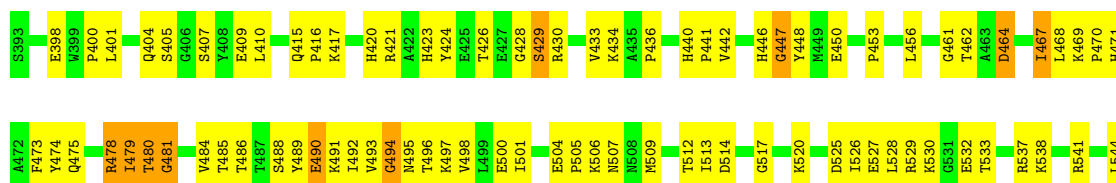
- Molecule 2: 5'-D(*TP*TP*TP*GP*GP*AP*AP*AP*GP*TP*CP*CP*CP*CP*A)-3'

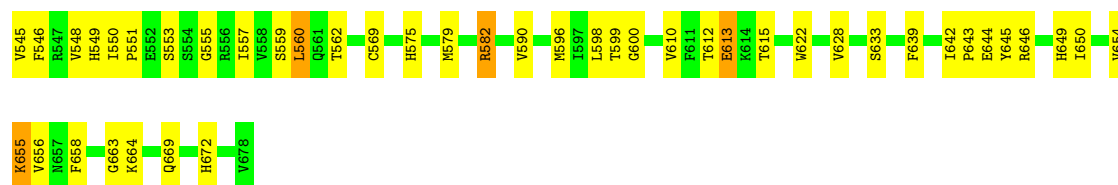
Chain D: 



- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

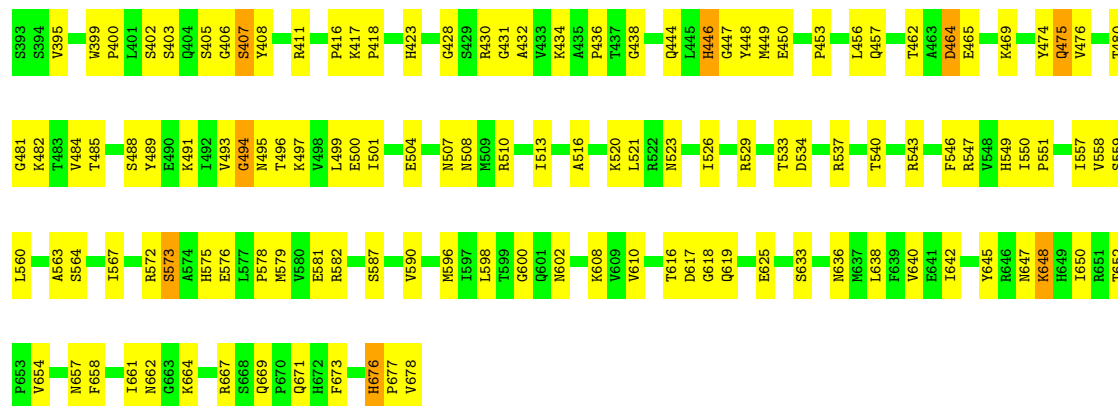
Chain L: 





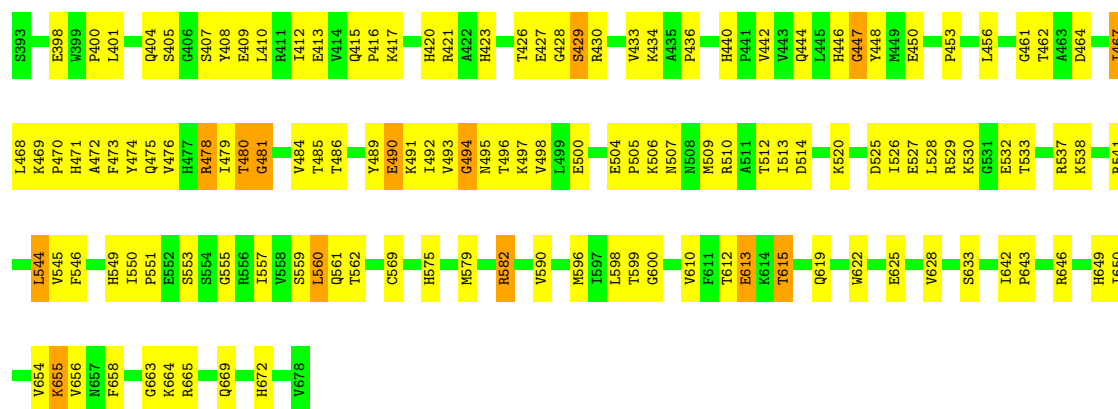
- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain M: 56% 41%



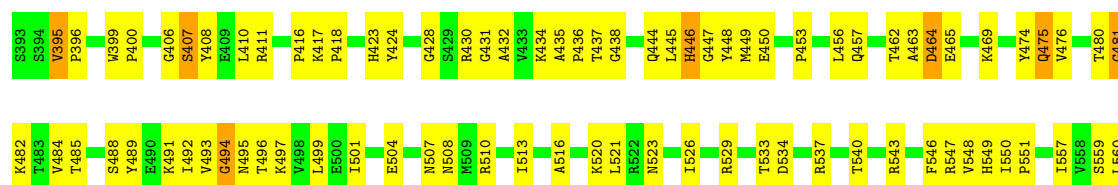
- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

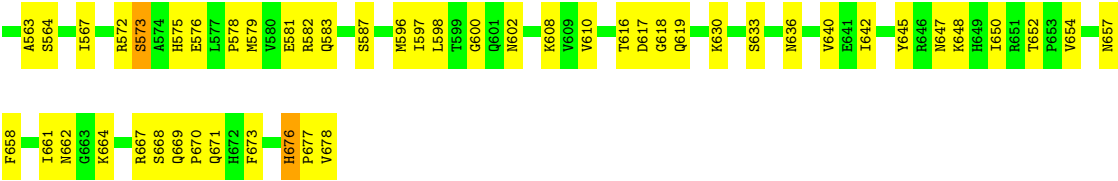
Chain N: 54% 41% 5%



- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain O: 54% 43%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 80.32Å 80.31Å 71.20° 78.97° 78.94°	Depositor
Resolution (Å)	29.68 – 2.60 29.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.68-2.60) 89.8 (29.68-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.265 0.228 , 0.262	Depositor DCC
R_{free} test set	4971 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.480 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10395	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	0/343	0.72	0/528
1	C	0.35	0/343	0.71	0/528
2	B	0.36	0/339	0.72	0/521
2	D	0.34	0/339	0.69	0/521
3	L	0.50	0/2297	0.95	2/3111 (0.1%)
3	M	0.94	1/2297 (0.0%)	1.31	19/3111 (0.6%)
3	N	0.50	0/2297	0.95	2/3111 (0.1%)
3	O	0.94	2/2297 (0.1%)	1.33	22/3111 (0.7%)
All	All	0.71	3/10552 (0.0%)	1.10	45/14542 (0.3%)

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	C	0	1
3	M	0	2
3	O	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	464	ASP	C-N	-36.86	0.82	1.33
3	M	464	ASP	C-N	-36.80	0.82	1.33
3	O	463	ALA	C-N	-5.04	1.26	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	464	ASP	O-C-N	-29.86	87.77	123.30
3	O	464	ASP	O-C-N	-29.84	87.79	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	464	ASP	CA-C-N	20.34	160.40	121.54
3	M	464	ASP	C-N-CA	20.34	160.40	121.54
3	O	464	ASP	CA-C-N	20.34	160.38	121.54
3	O	464	ASP	C-N-CA	20.34	160.38	121.54
3	O	573	SER	CB-CA-C	15.41	133.96	109.61
3	M	573	SER	CB-CA-C	15.40	133.94	109.61
3	M	573	SER	N-CA-C	-11.97	93.60	110.35
3	O	573	SER	N-CA-C	-11.93	93.65	110.35
3	O	446	HIS	N-CA-C	8.08	123.36	111.96
3	M	446	HIS	N-CA-C	8.05	123.31	111.96
3	O	395	VAL	N-CA-C	7.51	116.00	109.02
3	O	431	GLY	N-CA-C	7.22	121.06	112.33
3	O	476	VAL	N-CA-C	-7.16	102.12	110.21
3	M	431	GLY	N-CA-C	6.82	120.58	112.33
3	M	428	GLY	N-CA-C	-6.73	103.93	112.54
3	M	476	VAL	N-CA-C	-6.69	102.65	110.21
3	O	428	GLY	N-CA-C	-6.55	104.15	112.54
3	L	615	THR	N-CA-C	-6.37	101.04	110.46
3	N	615	THR	N-CA-C	-6.32	101.11	110.46
3	O	618	GLY	N-CA-C	5.91	122.89	115.21
3	M	618	GLY	N-CA-C	5.89	122.86	115.21
3	O	407	SER	N-CA-C	-5.75	106.03	113.16
3	N	550	ILE	N-CA-C	5.64	113.45	107.76
3	O	676	HIS	CA-C-N	5.62	125.61	120.21
3	O	676	HIS	C-N-CA	5.62	125.61	120.21
3	O	676	HIS	N-CA-C	5.56	117.99	110.31
3	M	407	SER	N-CA-C	-5.54	106.29	113.16
3	L	550	ILE	N-CA-C	5.52	113.34	107.76
3	M	676	HIS	N-CA-C	5.50	117.90	110.31
3	O	652	THR	CA-C-N	5.45	125.72	119.83
3	O	652	THR	C-N-CA	5.45	125.72	119.83
3	M	438	GLY	N-CA-C	-5.33	108.34	114.69
3	O	395	VAL	CB-CA-C	-5.28	105.83	111.00
3	M	676	HIS	CA-C-N	5.25	125.25	120.21
3	M	676	HIS	C-N-CA	5.25	125.25	120.21
3	M	540	THR	N-CA-C	5.20	118.65	112.72
3	O	540	THR	N-CA-C	5.19	118.64	112.72
3	M	652	THR	CA-C-N	5.18	125.43	119.83
3	M	652	THR	C-N-CA	5.18	125.43	119.83
3	O	411	ARG	N-CA-C	5.16	117.86	109.24
3	M	411	ARG	N-CA-C	5.15	117.85	109.24
3	O	445	LEU	N-CA-C	-5.10	100.93	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	438	GLY	N-CA-C	-5.01	108.73	114.69

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	5	DG	Sidechain
3	M	464	ASP	Peptide,Mainchain
3	O	464	ASP	Peptide,Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	306	0	171	18	0
1	C	306	0	171	35	0
2	B	303	0	171	12	0
2	D	303	0	171	15	0
3	L	2247	0	2211	130	0
3	M	2247	0	2210	122	0
3	N	2247	0	2211	143	0
3	O	2247	0	2210	121	0
4	A	6	0	0	8	0
4	B	3	0	0	3	0
4	C	11	0	0	27	0
4	D	7	0	0	13	0
4	L	41	0	0	36	0
4	M	40	0	0	47	0
4	N	41	0	0	52	0
4	O	40	0	0	35	0
All	All	10395	0	9526	580	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 29.

All (580) 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:O:578:PRO:HG3	4:O:74:HOH:O	1.19	1.28
3:M:578:PRO:HG3	4:M:140:HOH:O	1.26	1.27
3:N:579:MET:HG2	4:N:59:HOH:O	1.29	1.26
3:O:548:VAL:HG12	4:O:172:HOH:O	1.29	1.25
3:M:406:GLY:HA2	4:M:144:HOH:O	1.30	1.24
3:O:406:GLY:HA2	4:O:185:HOH:O	1.32	1.23
1:C:4:DG:H1'	4:C:47:HOH:O	1.42	1.18
2:D:2:DT:H6	4:D:97:HOH:O	1.26	1.18
3:L:471:HIS:HA	4:L:165:HOH:O	1.44	1.17
3:L:512:THR:HA	4:L:119:HOH:O	1.49	1.09
3:N:442:VAL:HG22	4:N:53:HOH:O	1.53	1.07
3:M:449:MET:HE3	4:M:115:HOH:O	1.51	1.07
3:N:551:PRO:HA	4:N:85:HOH:O	1.54	1.06
3:M:494:GLY:HA3	4:M:10:HOH:O	1.53	1.06
1:C:4:DG:H4'	4:C:136:HOH:O	1.54	1.05
3:O:494:GLY:HA3	4:O:25:HOH:O	1.55	1.05
3:O:449:MET:HE3	4:O:133:HOH:O	1.57	1.04
4:B:93:HOH:O	1:C:2:DA:H2	1.38	1.03
3:N:467:ILE:H	3:N:467:ILE:HD12	1.24	1.02
3:M:543:ARG:HD3	3:M:563:ALA:HB1	1.37	1.02
3:L:493:VAL:HG12	3:L:494:GLY:H	1.25	1.01
3:O:543:ARG:HD3	3:O:563:ALA:HB1	1.38	1.01
3:N:493:VAL:HG12	3:N:494:GLY:H	1.26	1.01
3:N:561:GLN:HB3	4:N:48:HOH:O	1.60	1.00
3:L:479:ILE:CB	4:L:138:HOH:O	2.10	0.98
2:B:1:DT:H2''	2:B:2:DT:H5'	1.45	0.98
3:L:467:ILE:HD12	3:L:467:ILE:H	1.26	0.97
2:D:2:DT:H5''	4:D:97:HOH:O	1.63	0.97
1:C:7:DG:C5'	4:C:159:HOH:O	2.12	0.96
3:O:494:GLY:C	4:O:5:HOH:O	2.06	0.95
3:N:625:GLU:HA	4:N:184:HOH:O	1.64	0.94
3:N:633:SER:CB	4:N:27:HOH:O	2.14	0.94
3:L:442:VAL:HG22	4:L:119:HOH:O	1.69	0.93
3:N:582:ARG:NH1	4:N:152:HOH:O	2.00	0.92
1:C:4:DG:C8	4:C:181:HOH:O	2.23	0.91
3:L:639:PHE:CE1	4:L:145:HOH:O	2.23	0.91
3:M:590:VAL:HB	4:M:83:HOH:O	1.69	0.91
3:L:633:SER:CB	4:L:44:HOH:O	2.19	0.90
3:N:596:MET:HE3	3:N:598:LEU:HD11	1.53	0.90
1:A:2:DA:H1'	1:A:3:DT:H5'	1.54	0.89
3:L:475:GLN:HE21	3:L:497:LYS:H	1.19	0.89
3:O:533:THR:HG22	3:O:534:ASP:H	1.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:533:THR:HG22	3:M:534:ASP:H	1.38	0.88
3:N:475:GLN:HE21	3:N:497:LYS:H	1.21	0.88
3:L:475:GLN:NE2	3:L:497:LYS:H	1.73	0.87
1:C:4:DG:C5'	4:C:32:HOH:O	2.22	0.87
2:D:2:DT:C5'	4:D:97:HOH:O	2.16	0.87
3:N:475:GLN:NE2	3:N:497:LYS:H	1.74	0.86
3:O:572:ARG:O	3:O:573:SER:C	2.19	0.85
3:O:493:VAL:N	4:O:155:HOH:O	2.09	0.85
3:N:541:ARG:CD	4:N:157:HOH:O	2.23	0.85
3:L:596:MET:HE3	3:L:598:LEU:HD11	1.58	0.85
3:L:423:HIS:CD2	3:L:429:SER:HA	2.12	0.85
3:L:655:LYS:HE3	3:L:656:VAL:O	1.76	0.85
3:N:541:ARG:NE	4:N:157:HOH:O	2.09	0.84
3:M:403:SER:N	4:M:167:HOH:O	2.10	0.84
3:N:423:HIS:CD2	3:N:429:SER:HA	2.13	0.84
3:O:583:GLN:HA	4:O:43:HOH:O	1.77	0.84
3:N:655:LYS:HE3	3:N:656:VAL:O	1.77	0.84
2:D:14:DC:H2''	2:D:15:DA:N7	1.93	0.83
3:M:572:ARG:O	3:M:573:SER:C	2.19	0.83
2:B:1:DT:H5''	2:D:15:DA:O3'	1.79	0.83
3:O:495:ASN:N	4:O:5:HOH:O	2.08	0.82
3:N:467:ILE:H	3:N:467:ILE:CD1	1.92	0.82
3:O:423:HIS:CD2	3:O:430:ARG:H	1.97	0.82
3:L:639:PHE:HE1	4:L:145:HOH:O	1.59	0.82
3:M:423:HIS:CD2	3:M:430:ARG:H	1.97	0.82
1:A:7:DG:H5'	4:A:112:HOH:O	1.80	0.82
3:L:493:VAL:HG12	3:L:494:GLY:N	1.95	0.81
3:O:489:TYR:HD2	3:O:499:LEU:HD11	1.46	0.81
3:M:494:GLY:C	4:M:24:HOH:O	2.23	0.81
3:N:493:VAL:HG12	3:N:494:GLY:N	1.96	0.81
3:N:610:VAL:HA	4:N:184:HOH:O	1.81	0.81
3:N:442:VAL:HG13	4:N:53:HOH:O	1.80	0.81
3:L:548:VAL:HB	4:L:154:HOH:O	1.81	0.80
3:L:557:ILE:HA	4:L:101:HOH:O	1.81	0.80
3:O:495:ASN:HB3	4:O:105:HOH:O	1.80	0.80
3:L:467:ILE:H	3:L:467:ILE:CD1	1.94	0.80
3:M:489:TYR:HD2	3:M:499:LEU:HD11	1.46	0.80
3:O:481:GLY:N	4:O:35:HOH:O	2.04	0.79
1:A:3:DT:H2''	1:A:4:DG:H5''	1.63	0.79
3:N:557:ILE:HA	4:N:85:HOH:O	1.80	0.79
3:L:551:PRO:HA	4:L:101:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:638:LEU:HB2	4:M:69:HOH:O	1.81	0.79
3:N:579:MET:CA	4:N:59:HOH:O	2.30	0.78
3:N:467:ILE:HD12	3:N:467:ILE:N	1.98	0.78
2:D:14:DC:C6	4:D:62:HOH:O	2.36	0.78
1:A:4:DG:N7	4:A:31:HOH:O	2.16	0.78
3:L:548:VAL:CB	4:L:154:HOH:O	2.32	0.77
3:N:474:TYR:CE1	3:N:520:LYS:HD3	2.19	0.77
3:L:474:TYR:CE1	3:L:520:LYS:HD3	2.20	0.77
3:L:548:VAL:CA	4:L:154:HOH:O	2.31	0.77
3:L:506:LYS:N	4:L:65:HOH:O	2.06	0.77
3:L:557:ILE:HG12	4:L:101:HOH:O	1.84	0.77
3:M:446:HIS:O	4:M:21:HOH:O	2.04	0.76
3:O:407:SER:OG	4:O:72:HOH:O	2.00	0.76
4:B:93:HOH:O	1:C:2:DA:C2	2.23	0.76
3:L:467:ILE:HD12	3:L:467:ILE:N	1.99	0.76
3:L:504:GLU:HB2	3:L:507:ASN:ND2	2.01	0.76
3:L:541:ARG:CD	4:L:162:HOH:O	2.33	0.76
3:O:493:VAL:HG13	4:O:155:HOH:O	1.84	0.76
3:N:504:GLU:HB2	3:N:507:ASN:ND2	2.00	0.76
3:M:638:LEU:HA	4:M:169:HOH:O	1.86	0.75
3:N:474:TYR:O	4:N:174:HOH:O	2.05	0.75
1:A:2:DA:H1'	1:A:3:DT:C5'	2.16	0.75
3:M:500:GLU:OE1	4:M:150:HOH:O	2.04	0.75
3:O:480:THR:CB	4:O:76:HOH:O	2.34	0.74
2:D:13:DC:H1'	4:D:135:HOH:O	1.87	0.74
3:M:664:LYS:O	3:M:664:LYS:HD3	1.87	0.74
1:C:11:DT:O4	4:C:128:HOH:O	2.05	0.74
3:N:410:LEU:HD23	3:N:562:THR:HG22	1.70	0.74
3:N:579:MET:CB	4:N:59:HOH:O	2.30	0.74
3:L:475:GLN:HE21	3:L:497:LYS:N	1.85	0.74
3:M:572:ARG:C	3:M:573:SER:O	2.29	0.74
1:C:4:DG:N3	4:C:47:HOH:O	2.21	0.73
3:L:549:HIS:N	4:L:154:HOH:O	2.14	0.73
3:M:662:ASN:N	4:M:140:HOH:O	2.20	0.73
3:O:664:LYS:O	3:O:664:LYS:HD3	1.88	0.73
3:L:541:ARG:NE	4:L:162:HOH:O	2.20	0.73
3:M:405:SER:HB3	4:M:13:HOH:O	1.88	0.73
3:M:494:GLY:HA2	4:M:24:HOH:O	1.88	0.73
2:D:13:DC:C1'	4:D:135:HOH:O	2.35	0.73
1:C:2:DA:H2''	1:C:3:DT:O5'	1.88	0.73
3:N:475:GLN:HE21	3:N:497:LYS:N	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:638:LEU:CB	4:M:69:HOH:O	2.37	0.72
3:O:492:ILE:C	4:O:155:HOH:O	2.33	0.72
3:O:597:ILE:O	4:O:43:HOH:O	2.07	0.72
3:L:493:VAL:CG1	3:L:494:GLY:H	2.02	0.72
3:N:493:VAL:CG1	3:N:494:GLY:H	2.02	0.72
3:L:410:LEU:HD23	3:L:562:THR:HG22	1.71	0.72
3:N:412:ILE:HB	4:N:179:HOH:O	1.87	0.72
3:M:495:ASN:N	4:M:24:HOH:O	2.21	0.72
3:M:480:THR:CB	4:M:56:HOH:O	2.37	0.71
3:N:471:HIS:HA	4:N:168:HOH:O	1.89	0.71
3:O:630:LYS:O	4:O:39:HOH:O	2.08	0.71
1:A:3:DT:C2'	1:A:4:DG:H5''	2.20	0.71
3:M:406:GLY:CA	4:M:144:HOH:O	2.07	0.71
3:L:447:GLY:N	4:L:16:HOH:O	2.08	0.71
3:N:428:GLY:N	4:N:156:HOH:O	2.05	0.71
3:M:494:GLY:CA	4:M:24:HOH:O	2.38	0.71
3:L:478:ARG:O	3:L:480:THR:N	2.23	0.71
1:A:9:DC:OP1	4:A:57:HOH:O	2.07	0.71
3:L:404:GLN:HB2	3:L:409:GLU:HG3	1.72	0.71
3:N:613:GLU:HG3	3:N:656:VAL:HG12	1.71	0.71
2:D:7:DA:O3'	4:D:19:HOH:O	2.09	0.71
1:C:7:DG:N3	4:C:117:HOH:O	2.23	0.70
1:C:12:DT:OP2	4:C:90:HOH:O	2.09	0.70
3:N:478:ARG:O	3:N:480:THR:N	2.24	0.70
1:C:7:DG:H5'	4:C:159:HOH:O	1.83	0.70
3:N:579:MET:HA	4:N:59:HOH:O	1.91	0.69
1:C:5:DG:H5''	4:C:129:HOH:O	1.93	0.69
3:L:613:GLU:HG3	3:L:656:VAL:HG12	1.74	0.69
3:N:404:GLN:HB2	3:N:409:GLU:HG3	1.74	0.69
3:L:442:VAL:HA	4:L:119:HOH:O	1.92	0.69
3:M:402:SER:HB2	4:M:167:HOH:O	1.91	0.69
3:O:573:SER:N	4:O:100:HOH:O	2.06	0.69
3:O:480:THR:O	3:O:482:LYS:N	2.27	0.68
3:O:633:SER:CB	4:O:39:HOH:O	2.40	0.68
2:D:2:DT:O3'	4:D:18:HOH:O	2.12	0.68
3:M:543:ARG:CD	3:M:563:ALA:HB1	2.19	0.68
1:C:4:DG:C4'	4:C:136:HOH:O	2.23	0.67
3:N:447:GLY:N	4:N:30:HOH:O	2.15	0.67
3:O:578:PRO:CG	4:O:74:HOH:O	2.01	0.67
2:B:1:DT:O2	4:B:93:HOH:O	2.11	0.67
3:M:480:THR:O	3:M:482:LYS:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:DG:O5'	4:C:159:HOH:O	2.10	0.67
3:N:510:ARG:NH2	4:N:78:HOH:O	2.02	0.66
3:N:553:SER:C	3:N:555:GLY:H	2.04	0.66
2:B:1:DT:H2''	2:B:2:DT:C5'	2.23	0.66
3:O:572:ARG:C	3:O:573:SER:O	2.29	0.66
3:M:457:GLN:CG	4:M:150:HOH:O	2.42	0.66
3:O:543:ARG:CD	3:O:563:ALA:HB1	2.19	0.66
2:D:2:DT:H1'	4:D:18:HOH:O	1.96	0.66
3:O:480:THR:HA	4:O:35:HOH:O	1.96	0.66
3:N:557:ILE:CG1	4:N:85:HOH:O	2.44	0.65
3:N:471:HIS:O	4:N:174:HOH:O	2.14	0.65
3:O:543:ARG:HD3	3:O:563:ALA:CB	2.21	0.65
3:L:417:LYS:HA	3:L:436:PRO:HG3	1.79	0.65
3:N:512:THR:HA	4:N:53:HOH:O	1.96	0.65
1:C:5:DG:C5'	4:C:129:HOH:O	2.44	0.65
3:L:462:THR:OG1	4:L:36:HOH:O	2.14	0.65
3:M:529:ARG:HB2	4:M:70:HOH:O	1.97	0.65
3:M:407:SER:O	3:M:447:GLY:HA3	1.96	0.65
3:M:667:ARG:CD	4:M:160:HOH:O	2.45	0.64
1:A:3:DT:H2''	1:A:4:DG:O4'	1.96	0.64
3:M:625:GLU:OE2	4:M:151:HOH:O	2.14	0.64
3:N:417:LYS:HA	3:N:436:PRO:HG3	1.78	0.64
3:O:407:SER:O	3:O:447:GLY:HA3	1.97	0.64
3:N:476:VAL:HG12	4:N:64:HOH:O	1.97	0.64
1:A:15:DA:C8	4:A:123:HOH:O	2.49	0.64
3:L:553:SER:C	3:L:555:GLY:H	2.04	0.64
3:N:528:LEU:HA	3:N:532:GLU:HB2	1.80	0.64
3:M:587:SER:HB3	3:M:676:HIS:HD2	1.63	0.64
3:L:528:LEU:HA	3:L:532:GLU:HB2	1.79	0.63
3:M:489:TYR:CD2	3:M:499:LEU:HD11	2.32	0.63
3:O:489:TYR:CD2	3:O:499:LEU:HD11	2.31	0.63
1:C:3:DT:H2''	1:C:4:DG:C8	2.34	0.63
3:M:543:ARG:HD3	3:M:563:ALA:CB	2.21	0.63
3:M:453:PRO:HB3	3:M:504:GLU:HG2	1.81	0.63
3:L:639:PHE:CD1	4:L:145:HOH:O	2.49	0.62
2:B:2:DT:H2''	2:B:3:DT:O5'	1.99	0.62
1:C:4:DG:H5'	4:C:32:HOH:O	1.95	0.62
3:M:457:GLN:HG2	4:M:150:HOH:O	1.99	0.62
3:N:453:PRO:HG3	3:N:505:PRO:CD	2.29	0.62
3:O:418:PRO:HA	4:O:130:HOH:O	1.99	0.62
3:N:622:TRP:CG	3:N:646:ARG:HD3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:622:TRP:CG	3:L:646:ARG:HD3	2.35	0.62
3:M:423:HIS:HD2	3:M:430:ARG:H	1.44	0.62
3:O:587:SER:HB3	3:O:676:HIS:HD2	1.65	0.62
3:L:453:PRO:HG3	3:L:505:PRO:CD	2.30	0.62
3:M:648:LYS:HA	4:M:83:HOH:O	1.99	0.62
3:N:575:HIS:CD2	3:N:663:GLY:HA3	2.35	0.62
3:L:575:HIS:CD2	3:L:663:GLY:HA3	2.35	0.61
3:L:633:SER:HA	4:L:145:HOH:O	1.99	0.61
3:M:526:ILE:O	3:M:529:ARG:HG2	2.01	0.61
3:O:526:ILE:O	3:O:529:ARG:HG2	2.00	0.61
1:C:4:DG:H2''	1:C:5:DG:C8	2.36	0.61
3:O:453:PRO:HB3	3:O:504:GLU:HG2	1.82	0.61
3:O:657:ASN:HA	3:O:671:GLN:O	2.01	0.61
3:O:423:HIS:HD2	3:O:430:ARG:H	1.44	0.61
2:D:8:DA:P	4:D:19:HOH:O	2.59	0.60
3:N:557:ILE:HG12	4:N:85:HOH:O	2.00	0.60
3:O:596:MET:HE3	3:O:598:LEU:HD11	1.82	0.60
4:C:42:HOH:O	3:N:664:LYS:HD2	2.01	0.60
3:M:462:THR:HG23	3:M:469:LYS:O	2.01	0.60
3:O:488:SER:O	3:O:501:ILE:HG22	2.02	0.60
3:M:657:ASN:HA	3:M:671:GLN:O	2.00	0.60
3:N:427:GLU:HB2	4:N:156:HOH:O	2.01	0.60
3:O:462:THR:HG23	3:O:469:LYS:O	2.02	0.59
3:L:420:HIS:O	3:L:569:CYS:HA	2.03	0.59
3:L:541:ARG:HD2	4:L:162:HOH:O	1.98	0.59
3:M:488:SER:O	3:M:501:ILE:HG22	2.01	0.59
3:L:471:HIS:CE1	3:L:473:PHE:HB2	2.37	0.59
3:N:412:ILE:CG2	4:N:179:HOH:O	2.49	0.59
3:N:471:HIS:CE1	3:N:473:PHE:HB2	2.38	0.59
3:N:420:HIS:O	3:N:569:CYS:HA	2.03	0.59
3:M:596:MET:HE3	3:M:598:LEU:HD11	1.85	0.59
3:M:572:ARG:HG3	4:M:149:HOH:O	2.02	0.58
3:N:481:GLY:HA2	3:N:485:THR:CB	2.33	0.58
3:M:638:LEU:CG	4:M:69:HOH:O	2.50	0.58
3:O:662:ASN:N	4:O:74:HOH:O	2.36	0.58
3:L:481:GLY:HA2	3:L:485:THR:CB	2.33	0.58
2:D:2:DT:C6	4:D:97:HOH:O	2.16	0.58
3:L:548:VAL:HA	4:L:154:HOH:O	2.02	0.58
1:C:12:DT:O5'	4:C:90:HOH:O	2.17	0.57
3:N:453:PRO:HG3	3:N:505:PRO:HD3	1.85	0.57
3:N:410:LEU:CD2	3:N:562:THR:HG22	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:453:PRO:HG3	3:L:505:PRO:HD3	1.86	0.57
3:N:448:TYR:CD2	3:N:509:MET:HE2	2.40	0.57
3:N:475:GLN:HG3	3:N:497:LYS:HB3	1.87	0.57
3:O:549:HIS:HD2	3:O:559:SER:OG	1.86	0.57
3:M:549:HIS:HD2	3:M:559:SER:OG	1.88	0.57
3:N:475:GLN:NE2	3:N:497:LYS:N	2.49	0.57
3:L:448:TYR:CD2	3:L:509:MET:HE2	2.40	0.57
3:M:638:LEU:HG	4:M:69:HOH:O	2.04	0.57
3:L:421:ARG:NH1	3:L:430:ARG:NH2	2.53	0.57
3:L:546:PHE:HB2	3:L:562:THR:HG23	1.86	0.57
3:L:475:GLN:HG3	3:L:497:LYS:HB3	1.86	0.56
1:A:6:DG:H1'	4:A:112:HOH:O	2.05	0.56
3:N:468:LEU:C	3:N:468:LEU:HD23	2.31	0.56
3:N:492:ILE:HG22	3:N:493:VAL:H	1.70	0.56
3:M:667:ARG:HG3	4:M:160:HOH:O	2.06	0.56
3:M:558:VAL:HA	4:M:71:HOH:O	2.05	0.56
3:N:546:PHE:HB2	3:N:562:THR:HG23	1.86	0.56
3:L:493:VAL:HG12	3:L:495:ASN:H	1.70	0.56
3:N:421:ARG:NH1	3:N:430:ARG:NH2	2.53	0.56
3:L:549:HIS:HD2	3:L:559:SER:OG	1.89	0.56
3:N:408:TYR:HA	4:N:30:HOH:O	2.05	0.55
3:L:448:TYR:CZ	3:L:450:GLU:HB2	2.41	0.55
3:N:446:HIS:O	4:N:142:HOH:O	2.18	0.55
3:L:468:LEU:HD23	3:L:468:LEU:C	2.32	0.55
3:N:448:TYR:CZ	3:N:450:GLU:HB2	2.41	0.55
3:L:410:LEU:CD2	3:L:562:THR:HG22	2.35	0.55
3:N:493:VAL:HG12	3:N:495:ASN:H	1.71	0.55
3:N:549:HIS:HD2	3:N:559:SER:OG	1.89	0.55
3:M:633:SER:HA	4:M:169:HOH:O	2.07	0.55
3:L:669:GLN:HE22	3:M:671:GLN:HE22	1.55	0.55
3:N:415:GLN:NE2	4:N:179:HOH:O	2.40	0.55
3:N:579:MET:HE2	3:O:669:GLN:HA	1.88	0.55
3:M:677:PRO:O	3:M:678:VAL:HB	2.07	0.54
3:N:655:LYS:NZ	3:N:672:HIS:ND1	2.46	0.54
3:L:492:ILE:HG22	3:L:493:VAL:H	1.71	0.54
3:M:456:LEU:HD11	3:M:546:PHE:HB3	1.89	0.54
3:N:412:ILE:CB	4:N:179:HOH:O	2.52	0.54
1:C:5:DG:H1'	1:C:6:DG:H5'	1.89	0.54
3:L:579:MET:HE2	3:M:669:GLN:HA	1.89	0.54
3:O:677:PRO:O	3:O:678:VAL:HB	2.07	0.54
3:L:417:LYS:HE2	3:L:434:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:475:GLN:HE22	3:L:496:THR:HA	1.73	0.54
3:L:475:GLN:NE2	3:L:497:LYS:N	2.48	0.53
3:N:669:GLN:HE22	3:O:671:GLN:HE22	1.57	0.53
3:O:482:LYS:HG3	3:O:485:THR:H	1.73	0.53
3:N:475:GLN:HE22	3:N:496:THR:HA	1.73	0.53
3:M:482:LYS:HG3	3:M:485:THR:H	1.73	0.53
1:C:12:DT:P	4:C:90:HOH:O	2.66	0.53
3:N:510:ARG:NE	4:N:78:HOH:O	2.39	0.53
3:O:456:LEU:HD11	3:O:546:PHE:HB3	1.89	0.53
3:M:475:GLN:NE2	3:M:496:THR:HA	2.23	0.53
3:L:464:ASP:OD1	4:L:36:HOH:O	2.19	0.53
3:O:617:ASP:OD2	3:O:619:GLN:HG3	2.08	0.53
1:C:4:DG:N7	4:C:181:HOH:O	2.36	0.52
3:N:417:LYS:HE2	3:N:434:LYS:HB2	1.91	0.52
3:O:475:GLN:NE2	3:O:496:THR:HA	2.24	0.52
3:O:583:GLN:CA	4:O:43:HOH:O	2.48	0.52
3:M:610:VAL:O	3:M:658:PHE:HA	2.10	0.52
3:N:505:PRO:HD2	4:N:127:HOH:O	2.08	0.52
3:M:510:ARG:O	3:M:510:ARG:HG3	2.09	0.52
3:O:494:GLY:C	3:O:496:THR:H	2.17	0.52
3:M:494:GLY:C	3:M:496:THR:H	2.18	0.52
3:O:493:VAL:HG22	4:O:155:HOH:O	2.09	0.52
3:O:610:VAL:O	3:O:658:PHE:HA	2.08	0.52
3:L:441:PRO:O	4:L:119:HOH:O	2.18	0.52
3:M:493:VAL:O	4:M:10:HOH:O	2.19	0.52
3:M:617:ASP:OD2	3:M:619:GLN:HG3	2.08	0.52
3:M:537:ARG:HG3	3:M:537:ARG:HH11	1.75	0.52
3:O:510:ARG:HG3	3:O:510:ARG:O	2.09	0.52
3:L:655:LYS:NZ	3:L:672:HIS:ND1	2.45	0.52
3:M:507:ASN:O	3:M:508:ASN:HB2	2.10	0.52
3:N:579:MET:CG	4:N:59:HOH:O	2.04	0.52
3:O:537:ARG:HG3	3:O:537:ARG:HH11	1.75	0.52
3:M:457:GLN:HG3	4:M:150:HOH:O	2.06	0.52
3:O:507:ASN:O	3:O:508:ASN:HB2	2.10	0.51
3:L:669:GLN:OE1	3:M:669:GLN:HG2	2.10	0.51
3:M:417:LYS:HG3	3:M:434:LYS:O	2.09	0.51
3:M:667:ARG:HD3	4:M:160:HOH:O	2.09	0.51
3:N:513:ILE:N	3:N:513:ILE:HD12	2.25	0.51
3:L:553:SER:C	3:L:555:GLY:N	2.68	0.51
3:M:596:MET:HG2	3:M:598:LEU:CD1	2.41	0.51
3:O:645:TYR:CZ	3:O:654:VAL:HG11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:513:ILE:HD12	3:L:513:ILE:N	2.26	0.51
3:N:442:VAL:CG2	4:N:53:HOH:O	2.32	0.51
2:B:5:DG:OP1	3:L:664:LYS:HG2	2.11	0.51
3:M:645:TYR:CZ	3:M:654:VAL:HG11	2.46	0.51
1:C:12:DT:H6	4:C:90:HOH:O	1.93	0.51
3:L:610:VAL:O	3:L:658:PHE:HA	2.11	0.51
3:M:480:THR:N	4:M:56:HOH:O	2.30	0.51
3:M:619:GLN:HA	4:M:186:HOH:O	2.10	0.51
3:O:417:LYS:HG3	3:O:434:LYS:O	2.10	0.51
3:O:474:TYR:CE1	3:O:520:LYS:HD3	2.46	0.51
3:O:480:THR:N	4:O:76:HOH:O	2.40	0.51
3:N:664:LYS:N	4:N:147:HOH:O	2.43	0.50
4:A:23:HOH:O	3:L:426:THR:HG23	2.09	0.50
3:N:553:SER:C	3:N:555:GLY:N	2.68	0.50
3:N:420:HIS:CD2	3:N:433:VAL:HA	2.46	0.50
2:B:3:DT:H1'	2:B:4:DG:C8	2.45	0.50
1:C:8:DA:O4'	4:C:117:HOH:O	2.19	0.50
3:L:505:PRO:HD2	4:L:65:HOH:O	2.11	0.50
3:N:409:GLU:N	4:N:30:HOH:O	2.08	0.50
3:L:420:HIS:CD2	3:L:433:VAL:HA	2.47	0.50
3:M:402:SER:CB	4:M:167:HOH:O	2.54	0.50
3:M:664:LYS:HD3	3:M:664:LYS:C	2.36	0.50
3:N:428:GLY:O	3:N:429:SER:C	2.54	0.50
3:N:492:ILE:HG22	3:N:493:VAL:N	2.26	0.50
3:N:513:ILE:HG22	4:N:92:HOH:O	2.11	0.50
3:O:596:MET:HG2	3:O:598:LEU:CD1	2.42	0.50
3:O:664:LYS:HD3	3:O:664:LYS:C	2.36	0.50
1:A:15:DA:N7	4:A:123:HOH:O	2.45	0.50
4:D:38:HOH:O	3:N:426:THR:HG23	2.12	0.50
3:L:462:THR:HG23	3:L:469:LYS:O	2.11	0.50
3:M:482:LYS:NZ	3:M:484:VAL:CB	2.74	0.50
3:L:492:ILE:HG22	3:L:493:VAL:N	2.27	0.50
3:M:474:TYR:CE1	3:M:520:LYS:HD3	2.47	0.50
3:N:461:GLY:HA2	3:N:470:PRO:HA	1.94	0.50
3:L:428:GLY:O	3:L:429:SER:C	2.54	0.50
3:M:418:PRO:HA	4:M:158:HOH:O	2.12	0.49
1:C:5:DG:O5'	4:C:129:HOH:O	2.20	0.49
3:M:449:MET:CE	4:M:115:HOH:O	2.31	0.49
3:O:482:LYS:HZ2	3:O:484:VAL:CB	2.25	0.49
3:O:533:THR:HG22	3:O:534:ASP:N	2.17	0.49
1:A:3:DT:C3'	1:A:4:DG:H5''	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:645:TYR:HA	4:L:146:HOH:O	2.11	0.49
3:O:482:LYS:NZ	3:O:484:VAL:CB	2.75	0.49
3:L:453:PRO:HG3	3:L:505:PRO:HD2	1.95	0.49
3:M:475:GLN:HE21	3:M:497:LYS:N	2.10	0.49
3:M:491:LYS:HD2	3:M:497:LYS:NZ	2.28	0.49
3:L:488:SER:CB	4:L:171:HOH:O	2.59	0.49
3:N:610:VAL:O	3:N:658:PHE:HA	2.13	0.49
3:L:525:ASP:O	3:L:529:ARG:HD3	2.12	0.49
3:L:579:MET:O	3:L:600:GLY:HA3	2.13	0.49
3:N:669:GLN:OE1	3:O:669:GLN:HG2	2.13	0.49
3:N:529:ARG:O	3:N:530:LYS:HB2	2.13	0.49
3:N:415:GLN:CD	4:N:179:HOH:O	2.56	0.49
3:N:453:PRO:HG3	3:N:505:PRO:HD2	1.95	0.49
3:O:492:ILE:CA	4:O:155:HOH:O	2.61	0.49
3:N:468:LEU:HD11	3:N:545:VAL:HG22	1.95	0.48
3:O:457:GLN:NE2	4:O:137:HOH:O	2.46	0.48
1:C:4:DG:H8	4:C:181:HOH:O	1.77	0.48
3:L:489:TYR:O	3:L:490:GLU:HB2	2.13	0.48
3:L:644:GLU:C	4:L:146:HOH:O	2.56	0.48
3:M:482:LYS:HZ2	3:M:484:VAL:CB	2.26	0.48
3:O:480:THR:CA	4:O:35:HOH:O	2.59	0.48
3:L:461:GLY:HA2	3:L:470:PRO:HA	1.95	0.48
3:M:533:THR:HG22	3:M:534:ASP:N	2.17	0.48
3:N:525:ASP:O	3:N:529:ARG:HD3	2.12	0.48
3:N:579:MET:O	3:N:600:GLY:HA3	2.12	0.48
3:L:529:ARG:O	3:L:530:LYS:HB2	2.13	0.48
3:O:395:VAL:HG13	3:O:399:TRP:CE3	2.49	0.48
3:L:628:VAL:CG1	4:L:44:HOH:O	2.61	0.48
3:M:638:LEU:HD23	4:M:169:HOH:O	2.14	0.48
3:L:622:TRP:CH2	4:L:146:HOH:O	2.67	0.48
3:M:581:GLU:C	3:M:582:ARG:HG3	2.39	0.48
3:O:642:ILE:HD13	3:O:673:PHE:CZ	2.49	0.48
3:N:442:VAL:CG1	4:N:53:HOH:O	2.51	0.48
3:O:475:GLN:HE21	3:O:497:LYS:N	2.11	0.48
3:L:468:LEU:HD11	3:L:545:VAL:HG22	1.95	0.47
3:M:408:TYR:HB2	4:M:13:HOH:O	2.13	0.47
3:M:457:GLN:O	3:M:546:PHE:HA	2.15	0.47
3:O:551:PRO:HA	3:O:557:ILE:HG22	1.96	0.47
3:O:581:GLU:C	3:O:582:ARG:HG3	2.39	0.47
1:A:12:DT:C7	3:L:424:TYR:CD1	2.97	0.47
3:L:407:SER:O	3:L:447:GLY:HA3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:608:LYS:HB2	3:O:661:ILE:HG22	1.96	0.47
2:B:5:DG:H5''	3:L:664:LYS:HG2	1.96	0.47
3:M:501:ILE:C	3:M:501:ILE:HD12	2.39	0.47
3:O:444:GLN:NE2	3:O:446:HIS:NE2	2.62	0.47
3:O:501:ILE:C	3:O:501:ILE:HD12	2.40	0.47
3:M:444:GLN:HE21	3:M:446:HIS:CE1	2.33	0.47
3:O:423:HIS:HB3	3:O:430:ARG:HB2	1.95	0.47
3:O:457:GLN:HB2	3:O:547:ARG:HB2	1.97	0.47
1:C:4:DG:O5'	4:C:32:HOH:O	2.20	0.47
3:M:513:ILE:HD12	3:M:513:ILE:H	1.80	0.47
3:N:407:SER:O	3:N:447:GLY:HA3	2.14	0.47
3:M:395:VAL:HG13	3:M:399:TRP:CE3	2.49	0.47
3:M:551:PRO:HA	3:M:557:ILE:HG22	1.96	0.47
3:N:462:THR:HG23	3:N:469:LYS:O	2.14	0.47
3:N:489:TYR:O	3:N:490:GLU:HB2	2.14	0.47
3:M:432:ALA:HA	3:M:516:ALA:O	2.14	0.47
3:O:444:GLN:HE21	3:O:446:HIS:CE1	2.33	0.47
3:O:491:LYS:HD2	3:O:497:LYS:NZ	2.30	0.47
3:L:415:GLN:OE1	3:L:416:PRO:HD2	2.15	0.47
3:M:608:LYS:HB2	3:M:661:ILE:HG22	1.97	0.46
3:O:513:ILE:HD12	3:O:513:ILE:H	1.81	0.46
1:A:2:DA:H1'	1:A:3:DT:O5'	2.15	0.46
3:N:446:HIS:O	3:N:448:TYR:N	2.48	0.46
3:N:484:VAL:O	3:N:486:THR:HG23	2.15	0.46
3:N:622:TRP:CD1	3:N:646:ARG:HD3	2.49	0.46
3:O:432:ALA:HA	3:O:516:ALA:O	2.15	0.46
3:L:484:VAL:O	3:L:486:THR:HG23	2.16	0.46
3:M:457:GLN:HB2	3:M:547:ARG:HB2	1.98	0.46
3:M:602:ASN:N	3:M:602:ASN:ND2	2.63	0.46
3:M:633:SER:CB	4:M:169:HOH:O	2.63	0.46
3:L:446:HIS:O	3:L:448:TYR:N	2.48	0.46
3:O:602:ASN:N	3:O:602:ASN:HD22	2.13	0.46
3:O:492:ILE:HA	4:O:155:HOH:O	2.16	0.46
3:O:602:ASN:N	3:O:602:ASN:ND2	2.62	0.46
3:M:642:ILE:HD13	3:M:673:PHE:CZ	2.50	0.46
3:N:415:GLN:OE1	3:N:416:PRO:HD2	2.15	0.46
3:M:444:GLN:NE2	3:M:446:HIS:NE2	2.63	0.46
3:N:472:ALA:N	4:N:168:HOH:O	2.12	0.46
2:B:5:DG:OP2	3:L:575:HIS:NE2	2.48	0.45
3:O:457:GLN:O	3:O:546:PHE:HA	2.16	0.45
3:O:533:THR:CG2	3:O:534:ASP:H	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:667:ARG:CD	4:O:96:HOH:O	2.64	0.45
2:D:8:DA:OP1	4:D:19:HOH:O	2.21	0.45
3:M:661:ILE:C	4:M:140:HOH:O	2.56	0.45
1:C:7:DG:P	4:C:159:HOH:O	2.75	0.45
3:L:649:HIS:O	3:L:650:ILE:C	2.60	0.45
3:M:608:LYS:HB2	3:M:661:ILE:CG2	2.47	0.45
3:N:412:ILE:HG21	4:N:179:HOH:O	2.12	0.45
3:M:489:TYR:HA	3:M:501:ILE:HG22	1.98	0.45
3:N:417:LYS:HG2	3:N:436:PRO:HA	1.99	0.45
3:N:658:PHE:CD1	3:N:658:PHE:C	2.94	0.45
3:O:410:LEU:HD12	3:O:410:LEU:HA	1.76	0.45
3:O:448:TYR:CZ	3:O:450:GLU:HB2	2.52	0.45
3:O:608:LYS:HB2	3:O:661:ILE:CG2	2.47	0.45
4:A:57:HOH:O	3:L:538:LYS:CE	2.65	0.44
3:M:423:HIS:HB3	3:M:430:ARG:HB2	1.98	0.44
3:O:489:TYR:HA	3:O:501:ILE:HG22	1.99	0.44
3:O:667:ARG:HD3	4:O:96:HOH:O	2.17	0.44
3:M:550:ILE:O	3:M:557:ILE:HA	2.17	0.44
3:M:600:GLY:O	3:M:636:ASN:HB2	2.18	0.44
3:O:406:GLY:CA	4:O:185:HOH:O	2.16	0.44
3:O:600:GLY:O	3:O:636:ASN:HB2	2.18	0.44
3:L:430:ARG:HG2	3:L:430:ARG:HH11	1.83	0.44
3:L:622:TRP:CD1	3:L:646:ARG:HD3	2.51	0.44
3:O:494:GLY:CA	4:O:5:HOH:O	2.54	0.44
3:O:550:ILE:O	3:O:557:ILE:HA	2.18	0.44
3:M:602:ASN:N	3:M:602:ASN:HD22	2.14	0.44
3:N:456:LEU:O	3:N:500:GLU:HA	2.17	0.44
3:N:541:ARG:HD2	4:N:157:HOH:O	2.02	0.44
3:O:543:ARG:HG3	3:O:564:SER:O	2.17	0.44
3:O:557:ILE:O	3:O:557:ILE:HG13	2.18	0.44
3:L:417:LYS:HG2	3:L:436:PRO:HA	1.99	0.44
3:L:596:MET:HG2	3:L:598:LEU:CD1	2.48	0.44
3:O:395:VAL:HA	3:O:396:PRO:HD3	1.89	0.44
3:O:576:GLU:OE1	3:O:576:GLU:HA	2.18	0.44
3:M:416:PRO:HG3	3:M:567:ILE:HD11	1.99	0.43
3:M:448:TYR:CZ	3:M:450:GLU:HB2	2.53	0.43
3:N:582:ARG:HD3	4:N:68:HOH:O	2.18	0.43
3:N:596:MET:HG2	3:N:598:LEU:CD1	2.48	0.43
3:L:475:GLN:NE2	3:L:496:THR:HA	2.33	0.43
3:O:520:LYS:NZ	3:O:523:ASN:ND2	2.66	0.43
1:C:10:DT:H71	4:C:128:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:557:ILE:CG1	4:L:101:HOH:O	2.56	0.43
3:L:658:PHE:CD1	3:L:658:PHE:C	2.95	0.43
3:M:638:LEU:N	4:M:69:HOH:O	2.51	0.43
3:N:610:VAL:HG22	4:N:184:HOH:O	2.18	0.43
3:N:642:ILE:HA	3:N:643:PRO:HD3	1.81	0.43
3:O:416:PRO:HG3	3:O:567:ILE:HD11	2.01	0.43
3:L:628:VAL:HG13	4:L:44:HOH:O	2.18	0.43
3:N:475:GLN:NE2	3:N:496:THR:HA	2.33	0.43
3:N:526:ILE:O	3:N:527:GLU:C	2.61	0.43
3:L:456:LEU:O	3:L:500:GLU:HA	2.18	0.43
3:N:582:ARG:HB2	3:N:599:THR:HB	2.01	0.43
2:B:8:DA:H2''	2:B:9:DG:OP2	2.17	0.43
1:C:1:DA:H2''	1:C:2:DA:O5'	2.19	0.43
3:L:669:GLN:HE22	3:M:671:GLN:NE2	2.17	0.43
3:N:665:ARG:N	4:N:147:HOH:O	2.14	0.43
3:O:578:PRO:HA	3:O:602:ASN:HB2	2.01	0.43
3:N:400:PRO:O	3:N:401:LEU:HD23	2.19	0.43
3:M:576:GLU:HA	3:M:576:GLU:OE1	2.18	0.43
3:N:444:GLN:NE2	4:N:78:HOH:O	2.52	0.42
3:L:504:GLU:HB2	3:L:507:ASN:HD22	1.79	0.42
3:L:622:TRP:NE1	3:L:646:ARG:HB3	2.33	0.42
3:M:543:ARG:HG3	3:M:564:SER:O	2.19	0.42
3:M:557:ILE:O	3:M:557:ILE:HG13	2.18	0.42
3:O:435:ALA:O	3:O:437:THR:N	2.52	0.42
3:N:423:HIS:HD1	3:N:423:HIS:H	1.68	0.42
3:N:537:ARG:O	3:N:538:LYS:HB2	2.20	0.42
3:N:557:ILE:CA	4:N:85:HOH:O	2.54	0.42
3:N:622:TRP:NE1	3:N:646:ARG:HB3	2.34	0.42
3:N:413:GLU:HG3	4:N:78:HOH:O	2.19	0.42
3:O:408:TYR:HB3	3:O:560:LEU:HD11	2.02	0.42
1:C:14:DC:H2''	1:C:15:DA:C8	2.54	0.42
3:L:582:ARG:HB2	3:L:599:THR:HB	2.02	0.42
3:L:612:THR:HA	3:L:622:TRP:O	2.20	0.42
3:M:578:PRO:HA	3:M:602:ASN:HB2	2.02	0.42
1:A:5:DG:H1'	1:A:6:DG:H5'	2.02	0.42
1:C:12:DT:C7	3:O:424:TYR:CD1	3.02	0.42
3:L:526:ILE:O	3:L:527:GLU:C	2.62	0.42
3:M:625:GLU:CG	4:M:151:HOH:O	2.67	0.42
3:N:579:MET:HE2	3:O:670:PRO:HD3	2.01	0.42
3:O:494:GLY:HA2	4:O:5:HOH:O	2.19	0.42
1:C:12:DT:H2'	4:C:90:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:520:LYS:NZ	3:O:523:ASN:HD21	2.18	0.42
3:L:410:LEU:HD12	3:L:410:LEU:HA	1.93	0.42
3:L:642:ILE:HA	3:L:643:PRO:HD3	1.81	0.42
3:O:579:MET:O	3:O:600:GLY:HA3	2.20	0.42
1:A:3:DT:H2''	1:A:4:DG:C5'	2.41	0.42
3:L:551:PRO:CA	4:L:101:HOH:O	2.53	0.42
2:B:4:DG:H2''	2:B:5:DG:O5'	2.20	0.41
3:N:430:ARG:HG2	3:N:430:ARG:HH11	1.85	0.41
3:N:612:THR:HA	3:N:622:TRP:O	2.20	0.41
3:N:615:THR:HG23	3:N:619:GLN:O	2.20	0.41
3:N:474:TYR:CZ	3:N:520:LYS:HD3	2.54	0.41
3:N:628:VAL:CG1	4:N:27:HOH:O	2.68	0.41
3:M:520:LYS:NZ	3:M:523:ASN:ND2	2.68	0.41
3:N:504:GLU:HB2	3:N:507:ASN:HD22	1.78	0.41
3:L:474:TYR:CZ	3:L:520:LYS:HD3	2.54	0.41
3:N:506:LYS:HG2	4:N:127:HOH:O	2.20	0.41
3:N:649:HIS:O	3:N:650:ILE:C	2.60	0.41
3:M:647:ASN:ND2	3:M:650:ILE:HG22	2.36	0.41
3:O:677:PRO:O	3:O:678:VAL:CB	2.69	0.41
3:M:579:MET:O	3:M:600:GLY:HA3	2.20	0.41
3:N:440:HIS:CD2	3:N:514:ASP:HB3	2.56	0.41
3:L:405:SER:HB2	3:L:560:LEU:HD11	2.03	0.41
3:L:440:HIS:CD2	3:L:514:ASP:HB3	2.56	0.41
3:L:456:LEU:HD11	3:L:546:PHE:HB3	2.03	0.41
3:L:537:ARG:O	3:L:538:LYS:HB2	2.21	0.41
3:N:544:LEU:HD23	3:N:546:PHE:CZ	2.55	0.41
3:O:435:ALA:C	3:O:437:THR:H	2.29	0.41
3:O:647:ASN:ND2	3:O:650:ILE:HG22	2.36	0.41
3:N:613:GLU:HB2	3:N:622:TRP:HB3	2.03	0.41
3:O:645:TYR:OH	3:O:654:VAL:HG11	2.21	0.41
3:L:456:LEU:HD23	3:L:501:ILE:HD11	2.03	0.40
3:N:504:GLU:HA	3:N:505:PRO:HD3	1.95	0.40
3:N:579:MET:HE1	3:O:668:SER:O	2.20	0.40
1:A:2:DA:H2''	1:A:3:DT:O5'	2.21	0.40
1:A:15:DA:C2	2:B:4:DG:N2	2.89	0.40
3:M:408:TYR:HB3	3:M:560:LEU:HD11	2.03	0.40
3:M:537:ARG:HG3	3:M:537:ARG:NH1	2.35	0.40
3:M:578:PRO:CG	4:M:140:HOH:O	2.12	0.40
3:O:417:LYS:HE3	3:O:434:LYS:HB2	2.04	0.40
3:L:517:GLY:N	4:L:138:HOH:O	2.54	0.40
3:O:537:ARG:HG3	3:O:537:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:DT:H2''	2:D:3:DT:C5'	2.51	0.40
3:L:410:LEU:HD22	3:L:548:VAL:HG22	2.04	0.40
3:L:400:PRO:O	3:L:401:LEU:HD23	2.22	0.40
3:L:430:ARG:HG2	3:L:430:ARG:NH1	2.37	0.40
3:N:405:SER:HB2	3:N:560:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	284/286 (99%)	245 (86%)	31 (11%)	8 (3%)	4	6
3	M	284/286 (99%)	247 (87%)	33 (12%)	4 (1%)	9	19
3	N	284/286 (99%)	245 (86%)	31 (11%)	8 (3%)	4	6
3	O	284/286 (99%)	246 (87%)	34 (12%)	4 (1%)	9	19
All	All	1136/1144 (99%)	983 (86%)	129 (11%)	24 (2%)	5	11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	479	ILE
3	M	465	GLU
3	M	481	GLY
3	N	479	ILE
3	O	465	GLU
3	O	481	GLY
3	L	447	GLY
3	L	481	GLY
3	N	447	GLY
3	N	481	GLY

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Mol	Chain	Res	Type
3	L	478	ARG
3	L	480	THR
3	L	490	GLU
3	M	494	GLY
3	N	480	THR
3	N	490	GLU
3	O	494	GLY
3	N	478	ARG
3	L	494	GLY
3	L	533	THR
3	N	494	GLY
3	N	533	THR
3	O	436	PRO
3	M	436	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	L	244/256 (95%)	231 (95%)	13 (5%)	20	43
3	M	244/256 (95%)	237 (97%)	7 (3%)	37	65
3	N	244/256 (95%)	231 (95%)	13 (5%)	20	43
3	O	244/256 (95%)	237 (97%)	7 (3%)	37	65
All	All	976/1024 (95%)	936 (96%)	40 (4%)	27	54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	398	GLU
3	L	429	SER
3	L	464	ASP
3	L	467	ILE
3	L	491	LYS
3	L	498	VAL
3	L	544	LEU

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Mol	Chain	Res	Type
3	L	560	LEU
3	L	582	ARG
3	L	590	VAL
3	L	613	GLU
3	L	654	VAL
3	L	655	LYS
3	M	400	PRO
3	M	475	GLN
3	M	521	LEU
3	M	575	HIS
3	M	616	THR
3	M	640	VAL
3	M	648	LYS
3	N	398	GLU
3	N	429	SER
3	N	464	ASP
3	N	467	ILE
3	N	491	LYS
3	N	498	VAL
3	N	544	LEU
3	N	560	LEU
3	N	582	ARG
3	N	590	VAL
3	N	613	GLU
3	N	654	VAL
3	N	655	LYS
3	O	400	PRO
3	O	475	GLN
3	O	521	LEU
3	O	575	HIS
3	O	616	THR
3	O	640	VAL
3	O	648	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	420	HIS
3	L	444	GLN
3	L	457	GLN
3	L	475	GLN
3	L	477	HIS

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Mol	Chain	Res	Type
3	L	507	ASN
3	L	508	ASN
3	L	539	ASN
3	L	549	HIS
3	L	601	GLN
3	L	657	ASN
3	L	671	GLN
3	M	404	GLN
3	M	420	HIS
3	M	423	HIS
3	M	440	HIS
3	M	444	GLN
3	M	457	GLN
3	M	475	GLN
3	M	495	ASN
3	M	507	ASN
3	M	523	ASN
3	M	539	ASN
3	M	549	HIS
3	M	565	ASN
3	M	571	GLN
3	M	575	HIS
3	M	583	GLN
3	M	602	ASN
3	M	647	ASN
3	M	662	ASN
3	M	671	GLN
3	M	676	HIS
3	N	420	HIS
3	N	444	GLN
3	N	457	GLN
3	N	475	GLN
3	N	477	HIS
3	N	507	ASN
3	N	508	ASN
3	N	539	ASN
3	N	549	HIS
3	N	601	GLN
3	N	657	ASN
3	N	671	GLN
3	O	404	GLN
3	O	420	HIS

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Mol	Chain	Res	Type
3	O	423	HIS
3	O	440	HIS
3	O	444	GLN
3	O	457	GLN
3	O	475	GLN
3	O	495	ASN
3	O	507	ASN
3	O	523	ASN
3	O	539	ASN
3	O	549	HIS
3	O	565	ASN
3	O	571	GLN
3	O	575	HIS
3	O	602	ASN
3	O	647	ASN
3	O	662	ASN
3	O	671	GLN
3	O	676	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	M	1
3	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	464:ASP	C	465:GLU	N	0.82
1	O	464:ASP	C	465:GLU	N	0.82

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	15/15 (100%)	-1.45	0 100 100	39, 56, 169, 180	0
1	C	15/15 (100%)	-1.57	0 100 100	40, 61, 102, 104	0
2	B	15/15 (100%)	-1.61	0 100 100	39, 57, 102, 168	0
2	D	15/15 (100%)	-1.54	0 100 100	39, 55, 132, 166	0
3	L	286/286 (100%)	-1.39	0 100 100	21, 48, 94, 130	0
3	M	286/286 (100%)	-1.45	0 100 100	25, 49, 89, 114	0
3	N	286/286 (100%)	-1.42	0 100 100	20, 49, 92, 130	0
3	O	286/286 (100%)	-1.45	0 100 100	25, 49, 95, 119	0
All	All	1204/1204 (100%)	-1.43	0 100 100	20, 49, 98, 180	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.