Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 12:58 AM EST

PDB ID	:	1P7H
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 (i) 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 (1)) were used in the production of this report:

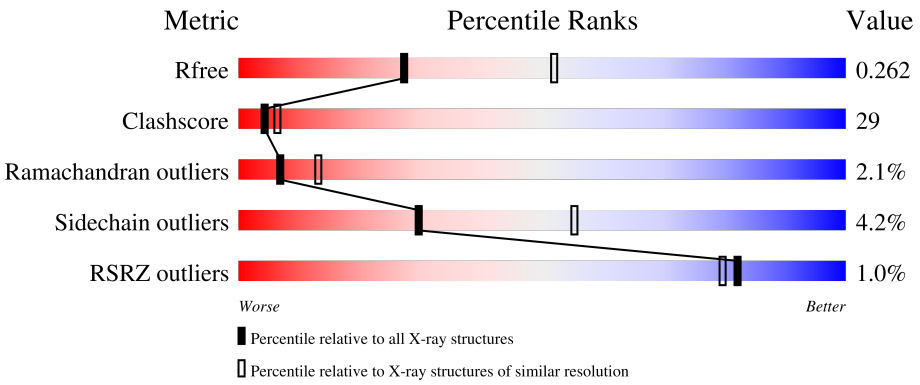
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	13%, 40%, 60%
1	C	15	13%, 80%, 7%
2	B	15	7%, 53%, 47%
2	D	15	7%, 53%, 47%
3	L	286	58%, 37%, 5%

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Mol	Chain	Length	Quality of chain
3	M	286	% 58% 40% •
3	N	286	57% 38% 5%
3	O	286	% 57% 41% •

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
			Total	C	N	O	P			
1	A	15	306	147	57	88	14	0	0	0
1	C	15	306	147	57	88	14	0	0	0

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

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

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

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

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.

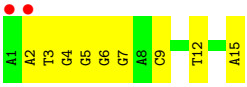
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	6	6	6	0	0
			Total	O		
4	B	3	3	3	0	0
			Total	O		
4	C	11	11	11	0	0
			Total	O		
4	D	7	7	7	0	0
			Total	O		
4	L	41	41	41	0	0
			Total	O		
4	M	40	40	40	0	0
			Total	O		
4	N	41	41	41	0	0
			Total	O		
4	O	40	40	40	0	0

3 Residue-property plots (i)

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

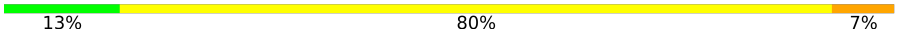
• Molecule 1: 5'-D(*AP*AP*TP*GP*GP*GP*GP*AP*CP*TP*TP*TP*CP*CP*A)-3'

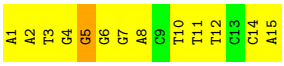
Chain A:



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

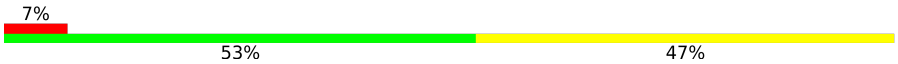
Chain C:

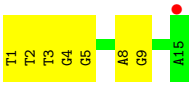




• Molecule 2: 5'-D(*TP*TP*TP*GP*GP*AP*AP*AP*GP*TP*CP*CP*CP*CP*A)-3'

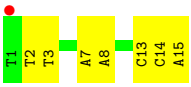
Chain B:





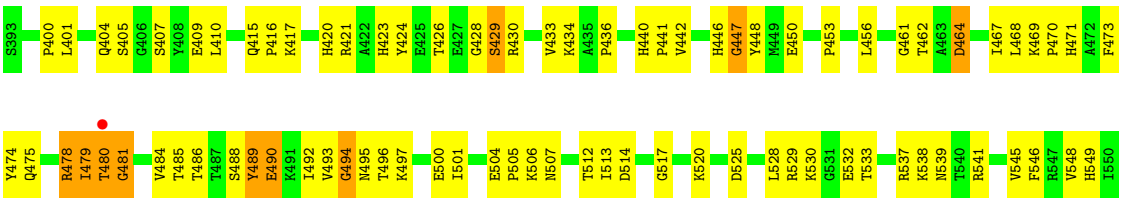
• Molecule 2: 5'-D(*TP*TP*TP*GP*GP*AP*AP*AP*GP*TP*CP*CP*CP*CP*A)-3'

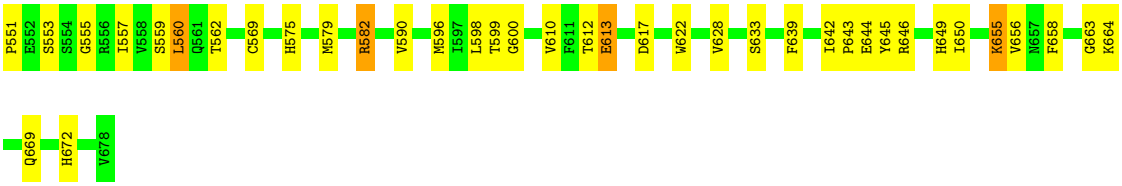
Chain D:



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

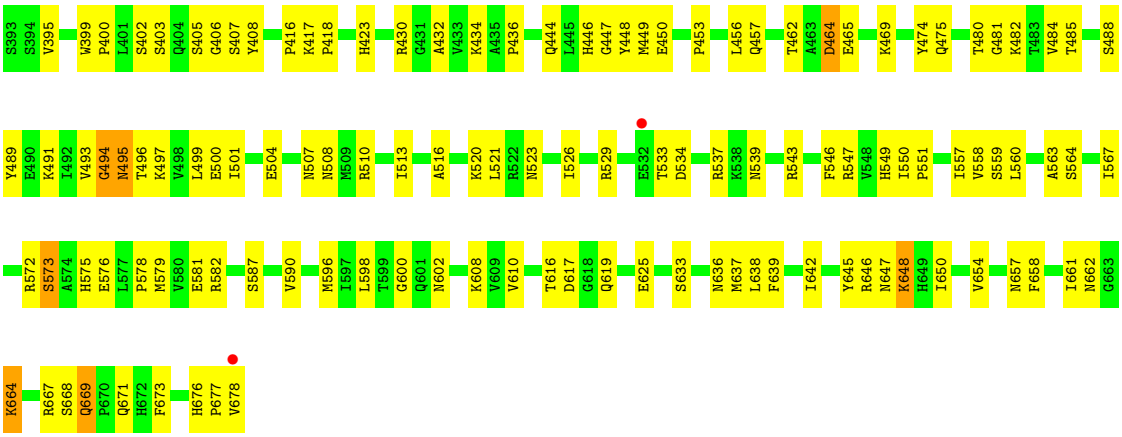
Chain L:





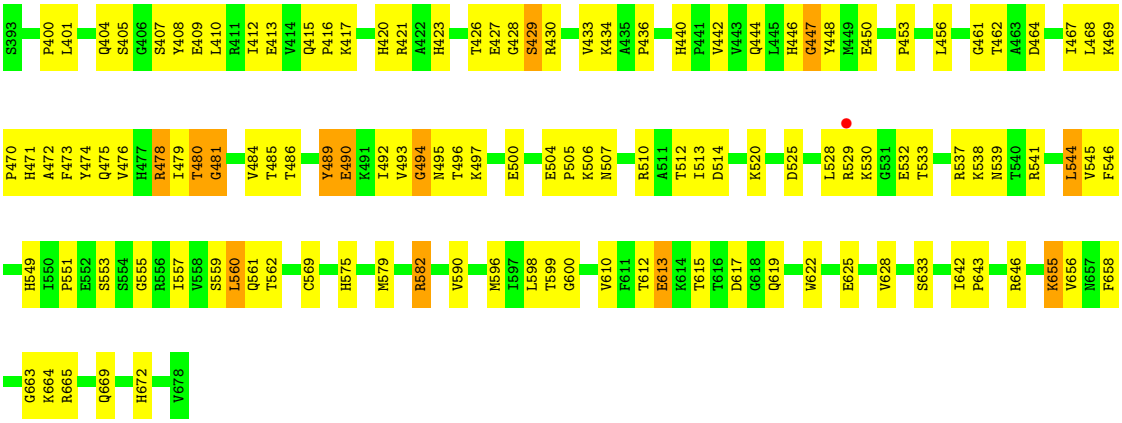
• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain M:



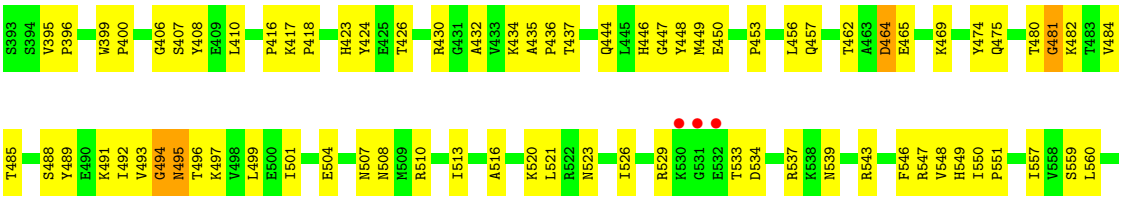
• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

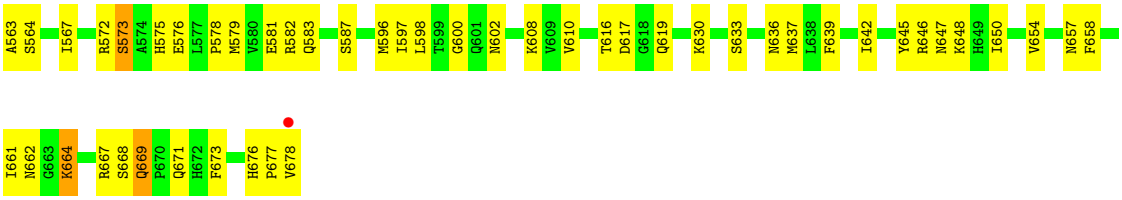
Chain N:



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

Chain O:




A563 S564 I567 R572 S573 A574 H575 E576 L577 P578 M579 V580 E581 R582 Q583 S587 M596 I597 L598 T599 G600 Q601 N602 K608 V609 V610 T616 D617 G618 Q619 K630 S633 N636 M637 L638 F639 I642 Y645 R646 N647 K648 H649 I650 V654 N657 F658
I661 N662 G663 K664 R667 S668 Q669 P670 Q671 H672 F673 H676 P677 V678

4 Data and refinement statistics (i)

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 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.68-2.60) 82.5 (29.68-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.32 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.480 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.93	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/343	0.74	0/528
1	C	0.53	0/343	0.72	0/528
2	B	0.55	0/339	0.74	0/521
2	D	0.46	0/339	0.70	0/521
3	L	0.41	0/2297	0.66	0/3111
3	M	0.65	1/2297 (0.0%)	0.92	5/3111 (0.2%)
3	N	0.40	0/2297	0.66	0/3111
3	O	0.65	1/2297 (0.0%)	0.92	5/3111 (0.2%)
All	All	0.54	2/10552 (0.0%)	0.79	10/14542 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	464	ASP	C-N	-22.59	0.82	1.34
3	M	464	ASP	C-N	-22.56	0.82	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	464	ASP	O-C-N	-21.83	87.77	122.70
3	O	464	ASP	O-C-N	-21.82	87.79	122.70
3	M	464	ASP	C-N-CA	15.48	160.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	464	ASP	C-N-CA	15.47	160.38	121.70
3	O	464	ASP	CA-C-N	14.47	149.04	117.20
3	M	464	ASP	CA-C-N	14.47	149.03	117.20
3	O	573	SER	CB-CA-C	12.56	133.96	110.10
3	M	573	SER	CB-CA-C	12.55	133.94	110.10
3	M	573	SER	N-CA-C	-6.45	93.60	111.00
3	O	573	SER	N-CA-C	-6.43	93.65	111.00

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	Mainchain,Peptide
3	O	464	ASP	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	306	0	171	19	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	129	0
3	M	2247	0	2210	122	0
3	N	2247	0	2211	138	0
3	O	2247	0	2210	122	0
4	A	6	0	0	8	0
4	B	3	0	0	3	0
4	C	11	0	0	28	0
4	D	7	0	0	13	0
4	L	41	0	0	35	0
4	M	40	0	0	46	0
4	N	41	0	0	53	0
4	O	40	0	0	35	0
All	All	10395	0	9526	577	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 (577) 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: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:O:494:GLY:C	4:O:5:HOH:O	2.06	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:633:SER:CB	4:L:44:HOH:O	2.19	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
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:495:ASN:N	4:O:5:HOH:O	2.08	0.86
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: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
2:B:1:DT:H5"	2:D:15:DA:O3'	1.79	0.83
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: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:O:572:ARG:O	3:O:573:SER:C	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:551:PRO:HA	4:L:101:HOH:O	1.80	0.79
3:M:572:ARG:O	3:M:573:SER:C	2.19	0.79
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:494:GLY:C	4:M:24:HOH:O	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:M:638:LEU:CB	4:M:69:HOH:O	2.37	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:M:572:ARG:C	3:M:573:SER:O	2.29	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
4:C:90:HOH:O	3:O:426:THR:OG1	2.10	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:1:DT:H2"	2:B:2:DT:C5'	2.23	0.66
3:M:457:GLN:CG	4:M:150:HOH:O	2.42	0.66
3:O:492:ILE:C	4:O:155:HOH:O	2.33	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: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: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:N:553:SER:C	3:N:555:GLY:H	2.04	0.61
3:O:572:ARG:C	3:O:573:SER:O	2.29	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
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:L:553:SER:C	3:L:555:GLY:H	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:410:LEU:CD2	3:N:562:THR:HG22	2.34	0.57
3:L:453:PRO:HG3	3:L:505:PRO:HD3	1.86	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: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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:520:LYS:HZ3	3:O:523:ASN:ND2	2.07	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: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:N:468:LEU:C	3:N:468:LEU:HD23	2.31	0.52
3:N:596:MET:CE	3:N:598:LEU:HD11	2.40	0.51
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:468:LEU:HD23	3:L:468:LEU:C	2.32	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: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
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:M:418:PRO:HA	4:M:158:HOH:O	2.12	0.49
3:O:520:LYS:HZ3	3:O:523:ASN:HD21	1.57	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: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
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:L:596:MET:CE	3:L:598:LEU:HD11	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:10:DT:H72	4:C:128:HOH:O	2.13	0.48
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: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:O:482:LYS:HZ2	3:O:484:VAL:CB	2.26	0.48
3:O:494:GLY:CA	4:O:5:HOH:O	2.54	0.48
3:O:602:ASN:N	3:O:602:ASN:ND2	2.62	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: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:494:GLY:C	3:O:496:THR:H	2.17	0.47
3:O:551:PRO:HA	3:O:557:ILE:HG22	1.96	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
3:M:494:GLY:C	3:M:496:THR:H	2.18	0.47
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:O:444:GLN:NE2	3:O:446:HIS:NE2	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:553:SER:C	3:L:555:GLY:N	2.68	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: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:M:664:LYS:HD3	3:M:664:LYS:C	2.36	0.45
3:N:428:GLY:O	3:N:429:SER:C	2.54	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
3:O:667:ARG:CD	4:O:96:HOH:O	2.64	0.45
3:O:664:LYS:HD3	3:O:664:LYS:C	2.36	0.45
2:D:8:DA:OP1	4:D:19:HOH:O	2.21	0.45
3:L:428:GLY:O	3:L:429:SER:C	2.54	0.45
1:C:7:DG:P	4:C:159:HOH:O	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N:553:SER:C	3:N:555:GLY:N	2.68	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:N:415:GLN:CD	4:N:179:HOH:O	2.56	0.44
3:O:550:ILE:O	3:O:557:ILE:HA	2.18	0.44
3:L:644:GLU:C	4:L:146:HOH:O	2.56	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:L:493:VAL:CG1	3:L:494:GLY:N	2.66	0.43
3:O:520:LYS:NZ	3:O:523:ASN:ND2	2.66	0.43
3:L:557:ILE:CG1	4:L:101:HOH:O	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:581:GLU:C	3:M:582:ARG:HG3	2.39	0.43
3:N:475:GLN:NE2	3:N:496:THR:HA	2.33	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:N:579:MET:HE1	3:O:668:SER:O	2.18	0.43
3:O:581:GLU:C	3:O:582:ARG:HG3	2.39	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:501:ILE:C	3:M:501:ILE:HD12	2.39	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:O:501:ILE:C	3:O:501:ILE:HD12	2.40	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:O:637:MET:HE1	3:O:639:PHE:CZ	2.54	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
3:N:579:MET:HE2	4:N:59:HOH:O	2.18	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:M:625:GLU:CG	4:M:151:HOH:O	2.67	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
3:M:637:MET:HE1	3:M:639:PHE:CZ	2.54	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:12:DT:H72	3:L:424:TYR:CD1	2.55	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:L:596:MET:HE3	3:L:598:LEU:HD11	2.03	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:647:ASN:ND2	3:O:650:ILE:HG22	2.36	0.41
3:M:520:LYS:HZ3	3:M:523:ASN:ND2	2.18	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
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:L:579:MET:HE1	3:M:668:SER:O	2.21	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
2:D:2:DT:H2"	2:D:3:DT:C5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:410:LEU:HD22	3:L:548:VAL:HG22	2.04	0.40
3:L:649:HIS:O	3:L:650:ILE:C	2.60	0.40
3:M:482:LYS:HZ2	3:M:484:VAL:CB	2.34	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
3:O:572:ARG:O	3:O:573:SER:O	2.39	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%)	5 7
3	M	284/286 (99%)	247 (87%)	33 (12%)	4 (1%)	11 22
3	N	284/286 (99%)	245 (86%)	31 (11%)	8 (3%)	5 7
3	O	284/286 (99%)	246 (87%)	34 (12%)	4 (1%)	11 22
All	All	1136/1144 (99%)	983 (86%)	129 (11%)	24 (2%)	7 13

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

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Mol	Chain	Res	Type
3	N	447	GLY
3	N	481	GLY
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 (i)

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%)	234 (96%)	10 (4%)	30	56
3	M	244/256 (95%)	234 (96%)	10 (4%)	30	56
3	N	244/256 (95%)	233 (96%)	11 (4%)	27	52
3	O	244/256 (95%)	234 (96%)	10 (4%)	30	56
All	All	976/1024 (95%)	935 (96%)	41 (4%)	30	55

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	429	SER
3	L	464	ASP
3	L	489	TYR
3	L	539	ASN
3	L	560	LEU

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Mol	Chain	Res	Type
3	L	582	ARG
3	L	590	VAL
3	L	613	GLU
3	L	617	ASP
3	L	655	LYS
3	M	400	PRO
3	M	495	ASN
3	M	521	LEU
3	M	539	ASN
3	M	575	HIS
3	M	616	THR
3	M	646	ARG
3	M	648	LYS
3	M	664	LYS
3	M	669	GLN
3	N	429	SER
3	N	464	ASP
3	N	489	TYR
3	N	539	ASN
3	N	544	LEU
3	N	560	LEU
3	N	582	ARG
3	N	590	VAL
3	N	613	GLU
3	N	617	ASP
3	N	655	LYS
3	O	400	PRO
3	O	495	ASN
3	O	521	LEU
3	O	539	ASN
3	O	575	HIS
3	O	616	THR
3	O	646	ARG
3	O	648	LYS
3	O	664	LYS
3	O	669	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	444	GLN
3	L	475	GLN

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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	M	404	GLN
3	M	423	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	571	GLN
3	M	583	GLN
3	M	602	ASN
3	M	662	ASN
3	M	671	GLN
3	M	676	HIS
3	N	444	GLN
3	N	475	GLN
3	N	507	ASN
3	N	508	ASN
3	N	539	ASN
3	N	549	HIS
3	N	601	GLN
3	O	404	GLN
3	O	423	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	571	GLN
3	O	583	GLN
3	O	602	ASN
3	O	662	ASN

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Mol	Chain	Res	Type
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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%)	0.08	2 (13%)	3	2	39, 56, 169, 180	0
1	C	15/15 (100%)	-0.45	0	100	100	40, 61, 102, 104	0
2	B	15/15 (100%)	-0.28	1 (6%)	17	13	39, 57, 102, 168	0
2	D	15/15 (100%)	-0.24	1 (6%)	17	13	39, 55, 132, 166	0
3	L	286/286 (100%)	-0.24	1 (0%)	94	93	21, 48, 94, 130	0
3	M	286/286 (100%)	-0.28	2 (0%)	87	86	25, 49, 89, 114	0
3	N	286/286 (100%)	-0.28	1 (0%)	94	93	20, 49, 92, 130	0
3	O	286/286 (100%)	-0.26	4 (1%)	75	71	25, 49, 95, 119	0
All	All	1204/1204 (100%)	-0.26	12 (0%)	82	80	20, 49, 98, 180	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	532	GLU	4.5
1	A	2	DA	4.2
1	A	1	DA	4.0
3	M	532	GLU	4.0
3	O	530	LYS	3.6
2	D	1	DT	3.5
3	O	678	VAL	3.1
2	B	15	DA	3.0
3	L	480	THR	2.4
3	O	531	GLY	2.3
3	M	678	VAL	2.3
3	N	529	ARG	2.0

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 monosaccharides 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.