



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:38 AM GMT

PDB ID : 2AJQ
Title : Structure of replicative DNA polymerase provides insights into the mechanisms for processivity, frameshifting and editing
Authors : Briebe, L.; Ellenberger, T.
Deposited on : 2005-08-02
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

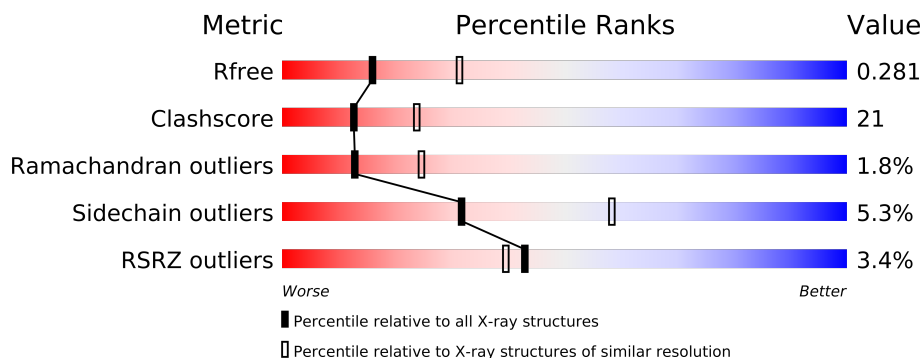
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	P	22	
1	X	22	
2	T	26	
2	Z	26	
3	A	704	
3	F	704	
4	B	108	
4	I	108	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14791 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	20	Total	C	N	O	P	0	0	1
			390	184	77	110	19			
1	X	21	Total	C	N	O	P	0	0	0
			432	204	87	120	21			

- Molecule 2 is a DNA chain called DNA Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	22	Total	C	N	O	P	0	0	0
			453	215	79	137	22			
2	Z	25	Total	C	N	O	P	0	0	0
			514	244	89	156	25			

- Molecule 3 is a protein called T7 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	704	Total	C	N	O	S	0	0	0
			5541	3527	971	1019	24			
3	F	689	Total	C	N	O	S	0	0	0
			5459	3480	953	1003	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	ASP	ENGINEERED	UNP P00581
A	7	ALA	GLU	ENGINEERED	UNP P00581
F	5	ALA	ASP	ENGINEERED	UNP P00581
F	7	ALA	GLU	ENGINEERED	UNP P00581

- Molecule 4 is a protein called thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total 799	C 517	N 129	O 150	S 3	0	0	0
4	I	105	Total 789	C 512	N 126	O 148	S 3	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	16	Total 16	O 16	0	0
5	T	21	Total 21	O 21	0	0
5	X	21	Total 21	O 21	0	0
5	Z	27	Total 27	O 27	0	0
5	A	158	Total 158	O 158	0	0
5	B	13	Total 13	O 13	0	0
5	F	142	Total 142	O 142	0	0
5	I	16	Total 16	O 16	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

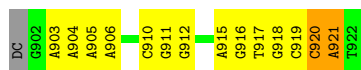
- Molecule 1: DNA Primer

Chain P: 



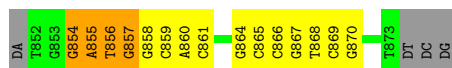
- Molecule 1: DNA Primer

Chain X: 



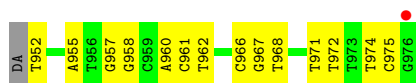
- Molecule 2: DNA Template

Chain T: 



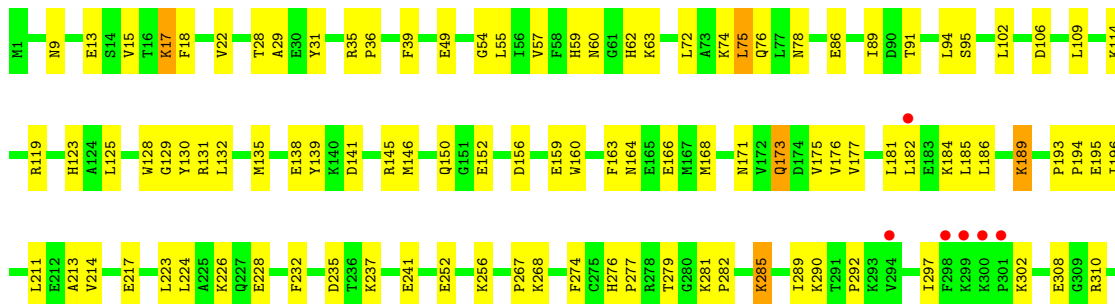
- Molecule 2: DNA Template

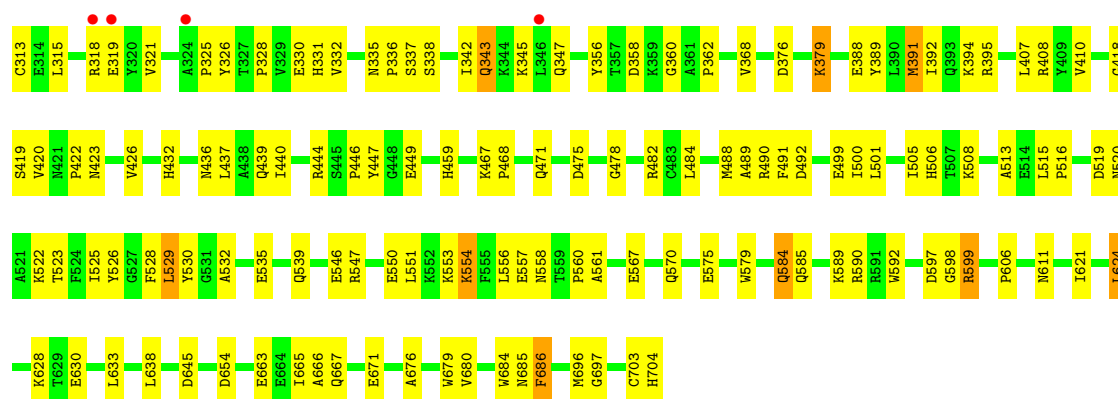
Chain Z: 



- Molecule 3: T7 DNA polymerase

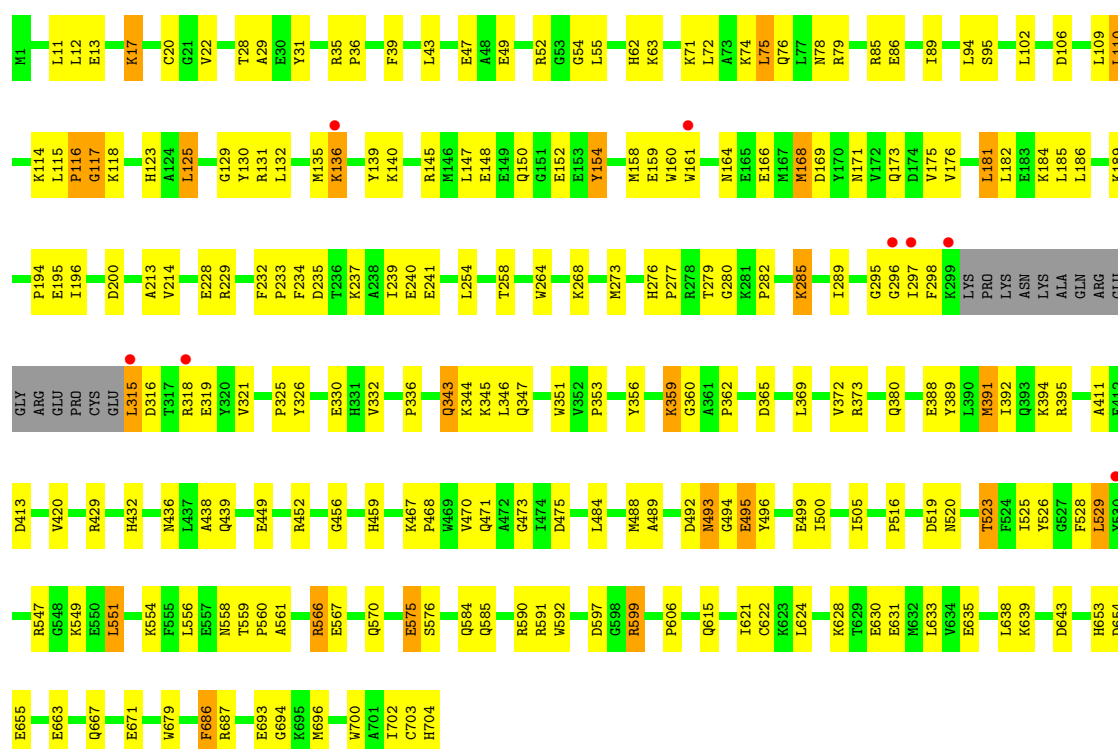
Chain A: 





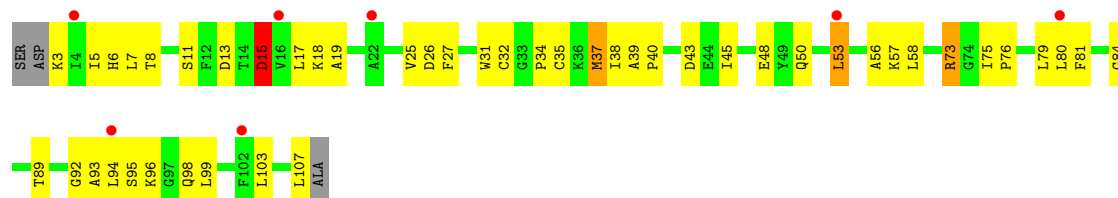
• Molecule 3: T7 DNA polymerase

Chain F:



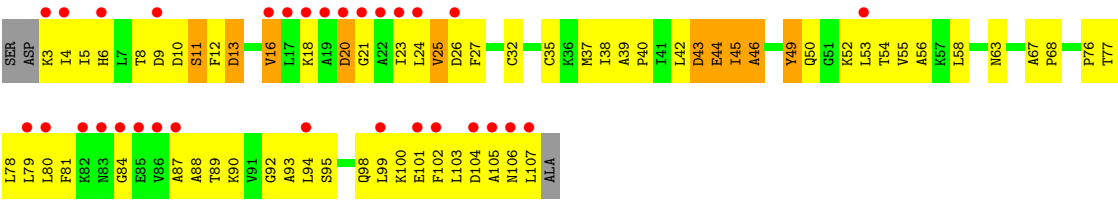
• Molecule 4: thioredoxin 1

Chain B:



• Molecule 4: thioredoxin 1

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	168.31Å 169.24Å 179.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.97 – 2.60 45.97 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.97-2.60) 95.7 (45.97-2.38)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.284 0.239 , 0.281	Depositor DCC
R_{free} test set	3929 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	EDS
Estimated twinning fraction	0.449 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 98459 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14791	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2DT

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	P	0.66	1/417 (0.2%)	0.90	1/642 (0.2%)
1	X	0.41	0/465	0.81	0/715
2	T	0.55	0/506	0.83	0/780
2	Z	0.46	0/574	0.77	0/885
3	A	0.39	0/5680	0.59	0/7693
3	F	0.39	0/5594	0.60	0/7570
4	B	0.31	0/814	0.55	0/1104
4	I	0.32	0/803	0.55	0/1089
All	All	0.40	1/14853 (0.0%)	0.63	1/20478 (0.0%)

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	P	0	2
1	X	0	2
2	T	0	4
2	Z	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	803	DA	O3'-P	-7.13	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	821	DA	N9-C1'-C2'	-5.54	102.08	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	820	DC	Sidechain
1	P	821	DA	Sidechain
2	T	854	DG	Sidechain
2	T	855	DA	Sidechain
2	T	856	DT	Sidechain
2	T	857	DG	Sidechain
1	X	920	DC	Sidechain
1	X	921	DA	Sidechain
2	Z	955	DA	Sidechain
2	Z	957	DG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	390	0	212	37	0
1	X	432	0	234	29	0
2	T	453	0	250	21	0
2	Z	514	0	284	13	0
3	A	5541	0	5382	186	0
3	F	5459	0	5338	179	0
4	B	799	0	814	45	0
4	I	789	0	794	92	0
5	A	158	0	0	14	0
5	B	13	0	0	1	0
5	F	142	0	0	7	1
5	I	16	0	0	4	0
5	P	16	0	0	0	0
5	T	21	0	0	0	0
5	X	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Z	27	0	0	0	0
All	All	14791	0	13308	577	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (577) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:73:ARG:HH11	4:B:73:ARG:HB3	1.11	1.09
2:T:867:DG:H2''	2:T:868:DT:H5'	1.32	1.07
4:I:16:VAL:HA	4:I:23:ILE:HG21	1.36	1.04
1:P:807:DC:H2''	1:P:808:DG:H5'	1.38	1.03
4:B:73:ARG:NH1	4:B:73:ARG:HB3	1.79	0.96
4:I:80:LEU:H	4:I:89:THR:HG22	1.31	0.94
1:X:917:DT:H2''	1:X:918:DG:H5'	1.50	0.93
4:I:25:VAL:HA	4:I:56:ALA:H	1.33	0.92
1:P:817:DT:H2''	1:P:818:DG:H5'	1.51	0.92
1:X:916:DG:H2''	1:X:917:DT:H5'	1.52	0.92
1:P:805:DA:H2''	1:P:806:DA:H5''	1.51	0.92
4:I:27:PHE:HE2	4:I:58:LEU:HD23	1.33	0.91
4:I:24:LEU:HD21	4:I:80:LEU:HD12	1.52	0.91
1:X:920:DC:H2''	1:X:921:DA:H5'	1.53	0.90
2:T:856:DT:H2''	2:T:857:DG:H5''	1.54	0.90
4:I:38:ILE:HD12	4:I:93:ALA:HA	1.54	0.89
4:B:27:PHE:HE2	4:B:58:LEU:HD23	1.37	0.89
3:F:321:VAL:HG21	4:I:94:LEU:HD21	1.55	0.89
4:B:38:ILE:HD12	4:B:93:ALA:HA	1.52	0.88
3:A:189:LYS:HG3	3:A:194:PRO:HG3	1.56	0.88
4:I:25:VAL:HG12	4:I:56:ALA:HB3	1.55	0.87
3:F:279:THR:HG22	3:F:280:GLY:H	1.37	0.86
4:I:24:LEU:HB2	4:I:55:VAL:HG22	1.57	0.85
1:X:920:DC:H2''	1:X:921:DA:C5'	2.07	0.85
4:I:24:LEU:HA	4:I:79:LEU:O	1.76	0.84
3:A:91:THR:HB	3:A:181:LEU:HD12	1.60	0.84
4:I:4:ILE:CG2	4:I:56:ALA:HA	2.08	0.83
3:F:164:ASN:OD1	3:F:166:GLU:HG2	1.78	0.83
3:F:315:LEU:HD23	3:F:316:ASP:H	1.44	0.83
3:A:321:VAL:HG21	4:B:94:LEU:HD21	1.61	0.83
4:I:24:LEU:CB	4:I:55:VAL:HG22	2.09	0.82
4:I:23:ILE:O	4:I:80:LEU:HA	1.79	0.82
1:X:921:DA:H8	1:X:921:DA:H5'	1.44	0.82
3:F:631:GLU:O	3:F:635:GLU:HG2	1.81	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:820:DC:H1'	5:A:5308:HOH:O	1.81	0.80
4:B:73:ARG:HH11	4:B:73:ARG:CB	1.93	0.80
4:B:27:PHE:HE1	4:B:79:LEU:HD22	1.47	0.79
2:T:856:DT:H2''	2:T:857:DG:C5'	2.12	0.79
4:I:12:PHE:HD1	4:I:13:ASP:H	1.30	0.79
3:A:276:HIS:HD2	3:A:279:THR:H	1.30	0.78
4:I:37:MET:O	4:I:40:PRO:HD2	1.81	0.78
2:Z:966:DC:H2''	2:Z:967:DG:C8	2.20	0.77
3:A:237:LYS:HA	3:A:237:LYS:HE2	1.67	0.77
3:A:22:VAL:HB	3:A:175:VAL:HG21	1.67	0.76
3:A:95:SER:OG	3:A:123:HIS:HD2	1.69	0.76
1:X:916:DG:H2''	1:X:917:DT:C5'	2.15	0.75
3:A:575:GLU:HG2	3:A:589:LYS:HG3	1.69	0.75
4:B:27:PHE:CE2	4:B:58:LEU:HD23	2.22	0.74
3:F:343:GLN:HG3	3:F:362:PRO:HG2	1.70	0.74
3:A:189:LYS:CG	3:A:194:PRO:HG3	2.17	0.74
3:A:436:ASN:HB3	3:A:439:GLN:HE21	1.53	0.74
3:F:55:LEU:HD13	3:F:89:ILE:HD11	1.70	0.74
3:F:63:LYS:HE3	3:F:228:GLU:OE2	1.88	0.73
3:F:72:LEU:HA	3:F:75:LEU:CD2	2.18	0.73
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.52	0.73
3:F:49:GLU:OE2	3:F:54:GLY:HA3	1.88	0.73
3:F:516:PRO:HG2	3:F:520:ASN:HD22	1.53	0.73
1:X:910:DC:H2''	1:X:911:DG:H5''	1.71	0.73
4:I:44:GLU:HG3	4:I:45:ILE:H	1.53	0.73
3:A:376:ASP:HB3	3:A:379:LYS:HB2	1.69	0.73
4:B:53:LEU:HD21	4:B:103:LEU:HD13	1.70	0.72
1:P:805:DA:C2'	1:P:806:DA:H5''	2.19	0.72
1:X:919:DC:H1'	3:F:394:LYS:HE2	1.70	0.72
3:A:189:LYS:N	3:A:189:LYS:HD2	2.04	0.72
3:A:484:LEU:HD22	3:A:529:LEU:HD21	1.71	0.72
3:A:343:GLN:HG2	3:A:347:GLN:HE21	1.54	0.72
4:I:4:ILE:HG21	4:I:56:ALA:HA	1.71	0.72
1:X:910:DC:H2''	1:X:911:DG:C5'	2.20	0.71
4:I:52:LYS:HD2	4:I:107:LEU:HD13	1.72	0.71
3:F:388:GLU:O	3:F:392:ILE:HG12	1.90	0.71
3:A:72:LEU:HA	3:A:75:LEU:HD11	1.72	0.71
3:A:318:ARG:HE	3:A:319:GLU:H	1.37	0.71
1:X:921:DA:C8	1:X:921:DA:H5'	2.25	0.71
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.71	0.71
3:F:95:SER:OG	3:F:123:HIS:HD2	1.73	0.70
3:A:585:GLN:HG2	5:A:5261:HOH:O	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:343:GLN:HG3	3:F:362:PRO:CG	2.21	0.70
1:P:807:DC:H2''	1:P:808:DG:C5'	2.20	0.70
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.20	0.70
2:T:858:DG:H2''	2:T:859:DC:H5'	1.73	0.70
4:B:37:MET:O	4:B:40:PRO:HD2	1.92	0.70
3:A:13:GLU:CD	3:A:13:GLU:H	1.96	0.70
4:I:27:PHE:CE2	4:I:58:LEU:HD23	2.21	0.69
3:F:273:MET:HG2	3:F:282:PRO:HB3	1.73	0.69
4:I:39:ALA:HB3	4:I:40:PRO:HD3	1.75	0.69
3:A:129:GLY:HA3	3:A:135:MET:HG2	1.74	0.69
3:A:528:PHE:HZ	3:A:556:LEU:HD21	1.58	0.69
3:F:13:GLU:CD	3:F:13:GLU:H	1.96	0.69
3:A:436:ASN:HB3	3:A:439:GLN:NE2	2.07	0.68
2:T:858:DG:H4'	3:A:432:HIS:O	1.92	0.68
3:F:575:GLU:HG3	3:F:576:SER:N	2.07	0.68
3:F:359:LYS:HE2	3:F:359:LYS:N	2.09	0.68
3:A:146:MET:HG2	3:A:150:GLN:HE21	1.57	0.68
3:A:128:TRP:CE3	3:A:131:ARG:HD2	2.28	0.68
4:I:79:LEU:HA	4:I:89:THR:HB	1.75	0.67
4:I:24:LEU:O	4:I:25:VAL:HG13	1.93	0.67
3:F:279:THR:HG22	3:F:280:GLY:N	2.09	0.67
3:F:484:LEU:HD22	3:F:529:LEU:HD21	1.76	0.67
3:A:519:ASP:O	3:A:523:THR:HG22	1.95	0.67
3:A:579:TRP:CE2	3:A:584:GLN:HG3	2.29	0.67
4:I:24:LEU:C	4:I:55:VAL:HA	2.16	0.66
3:F:519:ASP:O	3:F:523:THR:HG22	1.96	0.66
3:F:145:ARG:HA	3:F:148:GLU:HG2	1.76	0.66
3:A:276:HIS:CD2	3:A:279:THR:H	2.13	0.65
3:F:189:LYS:NZ	3:F:194:PRO:HB3	2.12	0.65
3:A:516:PRO:HG2	3:A:520:ASN:HD22	1.61	0.65
1:P:808:DG:H1	2:T:869:DC:H42	1.44	0.65
4:I:80:LEU:HB3	4:I:88:ALA:O	1.97	0.65
3:F:43:LEU:O	3:F:47:GLU:HG3	1.96	0.65
3:F:22:VAL:HB	3:F:175:VAL:HG21	1.78	0.64
4:I:88:ALA:HB1	4:I:106:ASN:CB	2.28	0.64
3:A:696:MET:HE3	5:A:5084:HOH:O	1.98	0.64
4:B:8:THR:HG22	4:B:11:SER:OG	1.96	0.64
3:F:663:GLU:HB2	3:F:696:MET:SD	2.38	0.64
3:A:330:GLU:HG3	3:A:332:VAL:HG13	1.80	0.64
4:I:8:THR:HA	4:I:63:ASN:HD21	1.62	0.64
3:F:516:PRO:HG2	3:F:520:ASN:ND2	2.12	0.64
3:F:547:ARG:NH1	3:F:551:LEU:HD13	2.12	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:297:ILE:HD12	3:A:297:ILE:N	2.12	0.64
4:B:27:PHE:CE1	4:B:79:LEU:HD22	2.32	0.64
3:A:388:GLU:O	3:A:392:ILE:HG12	1.98	0.63
3:A:91:THR:HB	3:A:181:LEU:CD1	2.28	0.63
3:F:110:LEU:HD21	3:F:117:GLY:HA2	1.80	0.63
3:A:194:PRO:HD2	3:A:195:GLU:OE2	1.98	0.63
3:A:553:LYS:O	3:A:557:GLU:HG3	1.99	0.63
3:F:285:LYS:HB3	3:F:285:LYS:NZ	2.14	0.63
4:I:58:LEU:HD11	4:I:63:ASN:ND2	2.14	0.63
4:B:79:LEU:HD23	4:B:81:PHE:HE1	1.64	0.63
2:T:856:DT:C2'	2:T:857:DG:H5''	2.28	0.62
3:F:633:LEU:HD22	3:F:638:LEU:HD12	1.80	0.62
3:F:336:PRO:HB2	3:F:389:TYR:CD1	2.33	0.62
3:A:135:MET:CE	3:A:173:GLN:HE22	2.12	0.62
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.81	0.62
3:A:489:ALA:HA	3:A:492:ASP:OD1	2.00	0.62
1:P:821:DA:H8	1:P:821:DA:H5'	1.63	0.62
3:A:516:PRO:HG2	3:A:520:ASN:ND2	2.15	0.62
1:P:820:DC:H2''	1:P:821:DA:OP2	1.99	0.62
4:I:24:LEU:HG	4:I:80:LEU:HB2	1.81	0.61
3:F:297:ILE:HD13	4:I:102:PHE:HA	1.82	0.61
4:B:26:ASP:OD2	4:B:57:LYS:HD2	2.00	0.61
3:A:345:LYS:HA	3:A:345:LYS:HE2	1.81	0.61
4:I:25:VAL:O	4:I:78:LEU:HA	2.01	0.61
4:I:46:ALA:HA	5:I:5005:HOH:O	1.99	0.61
3:F:189:LYS:HZ1	3:F:194:PRO:HB3	1.66	0.61
3:A:228:GLU:CD	3:A:419:SER:HA	2.19	0.61
3:F:321:VAL:HG22	4:I:90:LYS:HE3	1.81	0.61
4:B:53:LEU:HD12	4:B:53:LEU:C	2.21	0.61
4:B:8:THR:HG23	4:B:11:SER:H	1.64	0.61
3:A:55:LEU:HD13	3:A:89:ILE:HD11	1.83	0.61
3:A:146:MET:HG2	3:A:150:GLN:NE2	2.16	0.61
4:I:53:LEU:O	4:I:53:LEU:HD23	1.99	0.61
4:I:5:ILE:HG22	4:I:6:HIS:N	2.16	0.60
4:I:23:ILE:C	4:I:24:LEU:HD12	2.20	0.60
3:A:547:ARG:NH1	3:A:551:LEU:HD13	2.17	0.60
3:A:667:GLN:HE21	3:A:671:GLU:HG3	1.66	0.60
3:A:22:VAL:HG23	3:A:171:ASN:OD1	2.01	0.60
3:F:79:ARG:HD3	5:F:5018:HOH:O	2.00	0.60
3:F:184:LYS:O	3:F:184:LYS:HD3	2.02	0.60
2:T:867:DG:H2''	2:T:868:DT:C5'	2.19	0.60
1:P:812:DG:H2''	1:P:813:DC:H5''	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:439:GLN:HB2	5:A:5308:HOH:O	2.01	0.60
2:T:868:DT:H1'	2:T:869:DC:H5''	1.84	0.60
1:X:916:DG:H1'	1:X:917:DT:H5''	1.84	0.59
1:P:812:DG:H2''	1:P:813:DC:C5'	2.32	0.59
1:P:806:DA:H1'	1:P:807:DC:OP1	2.02	0.59
4:I:4:ILE:HG23	4:I:56:ALA:HA	1.83	0.59
3:F:148:GLU:C	3:F:150:GLN:H	2.06	0.59
4:B:13:ASP:HA	4:B:17:LEU:HD12	1.84	0.59
4:I:24:LEU:O	4:I:55:VAL:HA	2.02	0.59
4:I:26:ASP:N	4:I:56:ALA:O	2.33	0.59
3:A:285:LYS:HB3	3:A:285:LYS:NZ	2.18	0.59
3:F:496:TYR:O	3:F:500:ILE:HG12	2.03	0.59
3:A:315:LEU:H	3:A:315:LEU:HD23	1.67	0.59
3:F:28:THR:O	3:F:29:ALA:HB3	2.02	0.59
3:A:703:CYS:O	3:A:704:HIS:HB2	2.01	0.59
3:A:676:ALA:O	3:A:680:VAL:HG23	2.03	0.58
3:A:550:GLU:HG3	5:A:5421:HOH:O	2.03	0.58
3:F:289:ILE:HD12	3:F:325:PRO:HB2	1.84	0.58
1:P:807:DC:H5'	5:A:5117:HOH:O	2.04	0.58
3:F:484:LEU:O	3:F:488:MET:HG2	2.03	0.58
3:A:195:GLU:CD	3:A:195:GLU:H	2.06	0.58
4:I:5:ILE:HG22	4:I:6:HIS:H	1.69	0.58
4:B:79:LEU:HD12	4:B:89:THR:HB	1.85	0.58
3:A:391:MET:O	3:A:391:MET:HE2	2.03	0.58
3:F:136:LYS:HG3	3:F:173:GLN:HE21	1.69	0.58
4:B:11:SER:O	4:B:15:ASP:HB2	2.03	0.57
1:P:817:DT:H2''	1:P:818:DG:C5'	2.31	0.57
3:A:132:LEU:HD21	3:A:184:LYS:HG3	1.86	0.57
1:X:910:DC:C2'	1:X:911:DG:H5''	2.33	0.57
3:F:523:THR:HG21	5:F:5095:HOH:O	2.03	0.57
1:P:812:DG:C2'	1:P:813:DC:H5''	2.35	0.57
2:Z:974:DT:H2''	2:Z:975:DC:C5	2.39	0.57
3:A:289:ILE:HD12	3:A:325:PRO:HB2	1.85	0.57
3:A:228:GLU:HG2	3:A:418:GLY:O	2.03	0.57
4:I:95:SER:OG	4:I:98:GLN:HG3	2.05	0.57
3:A:467:LYS:HE3	3:A:468:PRO:HD2	1.86	0.57
1:X:903:DA:H2''	1:X:904:DA:N7	2.19	0.56
4:I:43:ASP:HB2	5:I:5012:HOH:O	2.05	0.56
3:A:500:ILE:HD13	3:A:505:ILE:HD13	1.87	0.56
4:I:32:CYS:HB3	4:I:35:CYS:HB2	1.87	0.56
3:F:94:LEU:HD21	3:F:214:VAL:HG13	1.87	0.56
3:F:173:GLN:O	3:F:176:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:816:DG:H1'	1:P:817:DT:H5''	1.86	0.56
3:A:109:LEU:HD22	3:A:114:LYS:HD3	1.88	0.56
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.05	0.56
4:B:79:LEU:HD23	4:B:81:PHE:CE1	2.41	0.56
3:F:547:ARG:HH12	3:F:551:LEU:HD13	1.71	0.56
3:A:130:TYR:CD1	3:A:135:MET:HG3	2.41	0.55
3:F:470:VAL:HG12	3:F:471:GLN:N	2.21	0.55
4:I:24:LEU:CA	4:I:79:LEU:O	2.51	0.55
3:A:513:ALA:HB3	3:A:515:LEU:HD23	1.87	0.55
2:T:869:DC:H2''	2:T:870:DG:C8	2.42	0.55
3:F:330:GLU:HG3	3:F:332:VAL:HG13	1.87	0.55
3:F:687:ARG:HH11	3:F:687:ARG:HB3	1.72	0.55
3:A:74:LYS:O	3:A:78:ASN:HA	2.07	0.55
2:Z:961:DC:H2'	2:Z:962:DT:H71	1.89	0.55
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.06	0.55
3:F:129:GLY:HA3	3:F:135:MET:HG2	1.89	0.55
3:A:138:GLU:HB2	3:A:141:ASP:OD2	2.07	0.55
3:F:74:LYS:O	3:F:78:ASN:HA	2.07	0.54
1:P:821:DA:C8	1:P:821:DA:H5'	2.41	0.54
3:F:429:ARG:HD2	3:F:615:GLN:NE2	2.23	0.54
1:X:917:DT:C2'	1:X:918:DG:H5'	2.31	0.54
3:F:639:LYS:NZ	3:F:643:ASP:OD1	2.40	0.54
3:F:489:ALA:HA	3:F:492:ASP:OD1	2.07	0.54
1:X:917:DT:H2''	1:X:918:DG:C5'	2.30	0.54
3:F:528:PHE:HZ	3:F:556:LEU:HD21	1.72	0.54
4:B:3:LYS:HD3	4:B:50:GLN:NE2	2.22	0.54
3:A:343:GLN:HG3	3:A:362:PRO:HG2	1.90	0.54
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.43	0.54
4:I:8:THR:CA	4:I:63:ASN:HD21	2.20	0.54
3:F:703:CYS:O	3:F:704:HIS:ND1	2.40	0.54
3:F:49:GLU:HA	3:F:52:ARG:NH1	2.23	0.54
4:I:44:GLU:HG3	4:I:45:ILE:N	2.21	0.54
1:X:915:DA:H2''	1:X:916:DG:H5'	1.88	0.53
3:A:224:LEU:HD12	3:A:422:PRO:HB3	1.88	0.53
3:F:129:GLY:C	3:F:135:MET:HG2	2.27	0.53
3:A:499:GLU:HG3	3:A:508:LYS:HE2	1.90	0.53
3:F:130:TYR:CD1	3:F:135:MET:HG3	2.43	0.53
3:F:585:GLN:HA	3:F:585:GLN:HE21	1.73	0.53
3:A:290:LYS:HD2	3:A:328:PRO:HG3	1.89	0.53
1:X:919:DC:C1'	3:F:394:LYS:HE2	2.37	0.53
3:A:376:ASP:OD2	3:A:379:LYS:HD3	2.08	0.53
3:F:235:ASP:HB2	3:F:459:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Z:971:DT:H2''	2:Z:972:DT:H71	1.89	0.53
1:P:807:DC:C2'	1:P:808:DG:H5'	2.27	0.53
1:P:821:DA:H2'	1:P:822:2DT:H73	1.91	0.53
3:A:106:ASP:CG	3:A:131:ARG:HH22	2.10	0.53
3:A:391:MET:C	3:A:391:MET:HE2	2.29	0.53
3:A:315:LEU:N	3:A:315:LEU:HD23	2.23	0.53
2:Z:960:DA:H2''	2:Z:961:DC:H5'	1.90	0.53
4:I:79:LEU:HD12	4:I:89:THR:HG21	1.90	0.53
1:P:809:DA:H1'	1:P:810:DC:H5'	1.91	0.53
4:I:16:VAL:CA	4:I:23:ILE:HG21	2.25	0.53
3:A:546:GLU:HB3	5:A:5202:HOH:O	2.07	0.53
1:P:805:DA:H2''	1:P:806:DA:O4'	2.09	0.53
3:A:290:LYS:HD3	3:A:326:TYR:OH	2.08	0.53
3:F:318:ARG:HH11	3:F:319:GLU:HG2	1.74	0.53
3:A:318:ARG:HE	3:A:319:GLU:N	2.05	0.52
3:A:528:PHE:CZ	3:A:556:LEU:HD21	2.42	0.52
3:F:467:LYS:HE3	3:F:468:PRO:HD2	1.91	0.52
4:B:75:ILE:HB	4:B:76:PRO:HA	1.92	0.52
2:Z:958:DG:H4'	3:F:432:HIS:O	2.09	0.52
3:F:35:ARG:HB3	3:F:36:PRO:HD2	1.90	0.52
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.90	0.52
3:F:700:TRP:HE1	3:F:704:HIS:CE1	2.26	0.52
3:F:268:LYS:HD2	3:F:330:GLU:CD	2.30	0.52
3:F:494:GLY:O	3:F:495:GLU:HB3	2.10	0.52
4:I:81:PHE:HB3	4:I:84:GLY:H	1.75	0.52
3:A:28:THR:O	3:A:29:ALA:HB3	2.10	0.52
4:B:39:ALA:N	4:B:40:PRO:CD	2.73	0.52
3:F:20:CYS:HB2	3:F:168:MET:CE	2.40	0.52
1:P:808:DG:H2''	1:P:809:DA:C8	2.45	0.52
3:A:666:ALA:HB3	3:A:696:MET:CE	2.40	0.51
3:A:492:ASP:HB3	3:A:561:ALA:HB2	1.91	0.51
3:A:164:ASN:OD1	3:A:166:GLU:HB2	2.09	0.51
3:F:181:LEU:HD22	3:F:185:LEU:HD11	1.92	0.51
4:B:38:ILE:HD12	4:B:93:ALA:CA	2.35	0.51
4:I:24:LEU:HB3	4:I:55:VAL:HG22	1.90	0.51
4:I:90:LYS:HD3	4:I:102:PHE:CZ	2.45	0.51
3:A:13:GLU:CD	3:A:13:GLU:N	2.64	0.51
3:F:116:PRO:O	3:F:118:LYS:N	2.43	0.51
4:B:40:PRO:HA	4:B:43:ASP:OD2	2.11	0.51
3:A:72:LEU:O	3:A:76:GLN:HB2	2.11	0.51
3:F:181:LEU:O	3:F:185:LEU:HG	2.11	0.51
4:I:49:TYR:CE2	4:I:103:LEU:HB3	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:338:SER:O	3:A:342:ILE:HG13	2.10	0.51
3:A:17:LYS:NZ	3:A:17:LYS:HB3	2.25	0.51
3:A:484:LEU:O	3:A:488:MET:HG2	2.11	0.50
3:F:567:GLU:HA	3:F:567:GLU:OE1	2.10	0.50
4:I:24:LEU:O	4:I:54:THR:O	2.29	0.50
4:B:5:ILE:HG22	4:B:6:HIS:O	2.11	0.50
3:A:321:VAL:CG2	4:B:94:LEU:HD21	2.39	0.50
3:F:132:LEU:HD21	3:F:184:LYS:HG3	1.93	0.50
3:F:687:ARG:NH1	3:F:687:ARG:HB3	2.26	0.50
2:T:865:DC:H2''	2:T:866:DC:O5'	2.11	0.50
3:A:331:HIS:HB3	5:A:5066:HOH:O	2.10	0.50
3:F:11:LEU:HB3	3:F:13:GLU:OE1	2.11	0.50
4:I:100:LYS:NZ	4:I:100:LYS:HB3	2.26	0.50
1:P:807:DC:H1'	1:P:808:DG:H5''	1.94	0.50
1:P:808:DG:H1	2:T:869:DC:N4	2.10	0.50
3:F:655:GLU:OE2	3:F:704:HIS:HE1	1.94	0.50
3:F:295:GLY:O	3:F:321:VAL:HA	2.12	0.50
3:F:391:MET:O	3:F:391:MET:HE2	2.11	0.50
4:I:107:LEU:HG	5:I:5013:HOH:O	2.12	0.50
3:A:624:LEU:HD12	3:A:684:TRP:CH2	2.47	0.50
3:A:135:MET:HE2	3:A:173:GLN:HE22	1.75	0.49
3:F:195:GLU:H	3:F:195:GLU:CD	2.14	0.49
2:T:864:DG:OP2	3:A:268:LYS:NZ	2.39	0.49
1:X:920:DC:H5'	3:F:394:LYS:HE3	1.94	0.49
3:F:315:LEU:CD2	3:F:316:ASP:H	2.19	0.49
3:F:590:ARG:HD2	3:F:592:TRP:O	2.12	0.49
3:A:478:GLY:O	3:A:482:ARG:HG3	2.12	0.49
3:F:139:TYR:CE2	3:F:159:GLU:HB2	2.47	0.49
4:I:37:MET:HG3	4:I:38:ILE:N	2.28	0.49
2:Z:960:DA:H2''	2:Z:961:DC:C5'	2.43	0.49
1:P:806:DA:H2''	1:P:807:DC:C5	2.47	0.49
3:A:141:ASP:O	3:A:145:ARG:HG2	2.11	0.49
4:B:25:VAL:HG22	4:B:56:ALA:HB3	1.94	0.49
4:I:80:LEU:HD23	4:I:80:LEU:C	2.33	0.49
3:A:129:GLY:CA	3:A:135:MET:HG2	2.41	0.49
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.42	0.49
3:F:452:ARG:HD2	5:F:5210:HOH:O	2.13	0.49
3:A:535:GLU:O	3:A:539:GLN:HG3	2.13	0.49
4:I:90:LYS:HD3	4:I:102:PHE:CE1	2.48	0.49
3:A:315:LEU:H	3:A:315:LEU:CD2	2.25	0.49
3:F:268:LYS:HD2	3:F:330:GLU:OE2	2.12	0.49
3:F:147:LEU:HD11	3:F:152:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:391:MET:HE1	3:A:392:ILE:HD13	1.94	0.48
3:F:298:PHE:CD2	3:F:315:LEU:HA	2.48	0.48
3:A:663:GLU:O	3:A:696:MET:HE1	2.13	0.48
3:A:102:LEU:HD12	3:A:123:HIS:CE1	2.48	0.48
4:I:52:LYS:CD	4:I:107:LEU:HD13	2.43	0.48
3:F:39:PHE:CZ	3:F:43:LEU:HD11	2.48	0.48
3:F:655:GLU:OE2	3:F:704:HIS:CE1	2.67	0.48
3:A:119:ARG:HH11	3:A:119:ARG:HG3	1.78	0.48
3:F:391:MET:CE	3:F:395:ARG:HG3	2.43	0.48
3:A:437:LEU:HA	3:A:440:ILE:CD1	2.42	0.48
3:F:200:ASP:HB2	5:F:5382:HOH:O	2.12	0.48
4:I:3:LYS:HE2	4:I:50:GLN:HE22	1.77	0.48
3:A:667:GLN:HE21	3:A:671:GLU:CG	2.25	0.48
3:A:408:ARG:HH11	3:A:408:ARG:HG2	1.78	0.48
2:T:868:DT:H2''	2:T:869:DC:C5'	2.44	0.48
4:I:102:PHE:C	4:I:104:ASP:H	2.15	0.48
4:I:24:LEU:HG	4:I:80:LEU:CB	2.43	0.48
4:B:37:MET:C	4:B:40:PRO:HD2	2.34	0.48
1:P:813:DC:H1'	1:P:814:DC:H5'	1.94	0.48
1:P:805:DA:H2''	1:P:806:DA:C5'	2.32	0.48
4:I:80:LEU:HD23	4:I:80:LEU:O	2.13	0.48
1:P:816:DG:H2''	1:P:817:DT:C5'	2.44	0.47
1:X:911:DG:H2''	1:X:912:DG:C8	2.49	0.47
3:F:494:GLY:O	3:F:495:GLU:CB	2.61	0.47
3:A:292:PRO:HA	5:A:5117:HOH:O	2.15	0.47
3:F:159:GLU:HG2	3:F:160:TRP:CD1	2.48	0.47
3:F:140:LYS:HE3	3:F:154:TYR:OH	2.14	0.47
1:P:805:DA:C3'	1:P:806:DA:H5''	2.45	0.47
4:I:9:ASP:N	4:I:63:ASN:HD21	2.13	0.47
3:A:128:TRP:CZ3	3:A:131:ARG:HD2	2.49	0.47
4:B:8:THR:HG23	4:B:11:SER:N	2.27	0.47
3:F:597:ASP:OD1	3:F:599:ARG:HD2	2.14	0.47
1:X:917:DT:H1'	1:X:918:DG:H5''	1.97	0.47
3:A:75:LEU:HD12	3:A:76:GLN:N	2.29	0.47
3:A:213:ALA:HA	3:A:597:ASP:OD2	2.15	0.47
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.95	0.47
3:A:9:ASN:HB3	3:A:17:LYS:HG3	1.97	0.47
3:F:570:GLN:HE22	3:F:606:PRO:HB3	1.80	0.47
3:A:35:ARG:HG3	3:A:35:ARG:HH11	1.79	0.47
3:F:556:LEU:HD11	3:F:566:ARG:NH2	2.30	0.47
1:P:816:DG:H2''	1:P:817:DT:H5'	1.96	0.46
3:F:72:LEU:HA	3:F:75:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:129:GLY:CA	3:F:135:MET:HG2	2.44	0.46
4:I:35:CYS:SG	4:I:76:PRO:HB3	2.56	0.46
2:T:854:DG:H5''	3:A:532:ALA:HA	1.97	0.46
3:A:114:LYS:HD2	5:A:5256:HOH:O	2.15	0.46
3:A:285:LYS:HB3	3:A:285:LYS:HZ3	1.79	0.46
1:X:916:DG:C2'	1:X:917:DT:C5'	2.89	0.46
2:T:854:DG:H2''	2:T:855:DA:H8	1.80	0.46
3:F:13:GLU:CD	3:F:13:GLU:N	2.63	0.46
3:F:549:LYS:HD3	5:F:5409:HOH:O	2.15	0.46
3:A:475:ASP:C	3:A:475:ASP:OD2	2.54	0.46
5:A:5435:HOH:O	3:F:240:GLU:HG3	2.16	0.46
4:I:9:ASP:N	4:I:63:ASN:ND2	2.64	0.46
4:I:44:GLU:CG	4:I:45:ILE:H	2.20	0.46
3:A:444:ARG:HB2	5:A:5161:HOH:O	2.16	0.46
3:A:109:LEU:CD2	3:A:114:LYS:HD3	2.45	0.46
3:F:31:TYR:CE2	3:F:176:VAL:HG12	2.50	0.46
3:F:318:ARG:NH1	3:F:319:GLU:HG2	2.30	0.46
3:A:159:GLU:HG2	3:A:160:TRP:CD1	2.50	0.46
3:A:31:TYR:OH	3:A:176:VAL:HG12	2.16	0.46
3:F:72:LEU:HA	3:F:75:LEU:HD21	1.94	0.46
3:F:115:LEU:O	3:F:117:GLY:N	2.36	0.46
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.98	0.46
4:I:8:THR:C	4:I:63:ASN:HD21	2.20	0.46
3:F:297:ILE:HD13	4:I:102:PHE:CA	2.46	0.46
1:P:820:DC:H5'	3:A:394:LYS:HE2	1.98	0.46
3:F:470:VAL:CG1	3:F:471:GLN:N	2.78	0.46
3:F:365:ASP:O	3:F:369:LEU:HB2	2.16	0.46
3:F:106:ASP:OD2	3:F:131:ARG:NH2	2.48	0.46
2:T:869:DC:H2''	2:T:870:DG:H8	1.81	0.45
3:F:315:LEU:HD23	4:I:105:ALA:HB1	1.97	0.45
3:F:136:LYS:CG	3:F:173:GLN:HE21	2.28	0.45
3:F:493:ASN:HD22	3:F:687:ARG:HH22	1.63	0.45
3:F:264:TRP:NE1	3:F:344:LYS:HE2	2.31	0.45
1:P:807:DC:H42	2:T:870:DG:H1	1.65	0.45
1:P:820:DC:C2'	1:P:821:DA:OP2	2.64	0.45
2:Z:966:DC:H2''	2:Z:967:DG:H8	1.76	0.45
4:B:45:ILE:HG13	4:B:99:LEU:CD1	2.46	0.45
3:F:693:GLU:HA	3:F:693:GLU:OE2	2.16	0.45
3:A:75:LEU:HD12	3:A:76:GLN:H	1.81	0.45
3:A:163:PHE:HE1	3:A:168:MET:HB2	1.80	0.45
3:F:351:TRP:CZ3	3:F:353:PRO:HG3	2.51	0.45
3:F:667:GLN:HE21	3:F:671:GLU:HG3	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:32:CYS:HB3	4:B:35:CYS:HB2	1.99	0.45
4:I:25:VAL:N	4:I:55:VAL:HG13	2.32	0.45
4:I:44:GLU:O	4:I:46:ALA:N	2.49	0.45
3:F:436:ASN:OD1	3:F:438:ALA:HB3	2.17	0.45
3:F:628:LYS:HE2	3:F:679:TRP:CD2	2.51	0.45
4:I:4:ILE:HG12	5:I:5003:HOH:O	2.16	0.45
3:A:59:HIS:O	3:A:60:ASN:HB3	2.17	0.45
3:F:449:GLU:HB3	5:F:5043:HOH:O	2.16	0.45
4:B:53:LEU:CD2	4:B:103:LEU:HD22	2.47	0.45
3:A:285:LYS:HG2	5:A:5041:HOH:O	2.17	0.45
3:F:168:MET:O	3:F:168:MET:HG3	2.17	0.45
2:T:867:DG:C2'	2:T:868:DT:H5'	2.23	0.45
3:A:547:ARG:O	3:A:551:LEU:HB2	2.17	0.44
3:F:496:TYR:CZ	3:F:505:ILE:HD11	2.52	0.44
4:B:95:SER:OG	4:B:98:GLN:HG3	2.17	0.44
4:I:44:GLU:CG	4:I:45:ILE:N	2.79	0.44
1:P:812:DG:H1'	1:P:813:DC:H5''	1.99	0.44
3:F:276:HIS:HA	3:F:277:PRO:HD3	1.88	0.44
2:T:860:DA:H2''	2:T:861:DC:H5'	1.99	0.44
1:X:921:DA:O4'	3:F:439:GLN:HA	2.16	0.44
3:A:181:LEU:O	3:A:185:LEU:HG	2.17	0.44
3:A:146:MET:O	3:A:150:GLN:HG3	2.18	0.44
3:F:326:TYR:HB3	4:I:92:GLY:HA2	1.98	0.44
3:F:298:PHE:HA	3:F:315:LEU:C	2.38	0.44
1:X:903:DA:H2''	1:X:904:DA:C8	2.52	0.44
3:F:473:GLY:HA3	3:F:703:CYS:HB3	2.00	0.44
3:A:94:LEU:HD21	3:A:214:VAL:HG13	1.99	0.44
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.84	0.44
3:A:525:ILE:HG23	3:A:526:TYR:N	2.32	0.44
3:F:234:PHE:CZ	3:F:239:ILE:HG13	2.53	0.44
3:A:335:ASN:OD1	3:A:337:SER:HB2	2.17	0.44
1:X:910:DC:H2''	1:X:911:DG:H5'	1.94	0.44
4:I:42:LEU:O	4:I:43:ASP:CB	2.66	0.44
3:F:585:GLN:HA	3:F:585:GLN:NE2	2.31	0.44
3:A:267:PRO:HD3	4:B:31:TRP:CZ3	2.53	0.44
4:I:67:ALA:HB3	4:I:68:PRO:HD3	1.99	0.44
4:I:99:LEU:O	4:I:99:LEU:HD23	2.18	0.44
3:F:71:LYS:O	3:F:75:LEU:HD22	2.17	0.43
3:A:63:LYS:HE2	3:A:228:GLU:OE1	2.18	0.43
3:A:106:ASP:HA	3:A:109:LEU:HD12	2.00	0.43
3:F:28:THR:O	3:F:29:ALA:CB	2.66	0.43
3:F:12:LEU:HD21	3:F:229:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:318:ARG:NH1	3:A:319:GLU:HG2	2.33	0.43
3:A:135:MET:HE1	3:A:173:GLN:HE22	1.82	0.43
3:F:31:TYR:N	3:F:31:TYR:CD1	2.87	0.43
3:A:407:LEU:HD23	3:A:407:LEU:HA	1.83	0.43
3:F:622:CYS:SG	3:F:654:ASP:HA	2.59	0.43
3:A:391:MET:HE3	3:A:395:ARG:HG3	1.99	0.43
3:A:235:ASP:HB2	3:A:459:HIS:CE1	2.54	0.43
3:A:18:PHE:CD2	3:A:39:PHE:HB2	2.53	0.43
1:X:904:DA:H2"	1:X:905:DA:C8	2.54	0.43
3:A:506:HIS:CG	3:A:522:LYS:HG2	2.54	0.43
4:B:107:LEU:HB2	5:B:5187:HOH:O	2.18	0.43
3:A:252:GLU:HG3	3:A:256:LYS:NZ	2.33	0.43
3:F:373:ARG:HA	3:F:380:GLN:OE1	2.18	0.43
3:F:233:PRO:HB2	3:F:456:GLY:O	2.18	0.43
3:A:135:MET:HA	3:A:135:MET:HE2	2.01	0.43
3:A:17:LYS:HB3	3:A:17:LYS:HZ3	1.83	0.43
3:A:281:LYS:HA	3:A:282:PRO:HD3	1.93	0.43
1:P:806:DA:H2"	1:P:807:DC:C6	2.54	0.43
3:A:488:MET:HB2	3:A:561:ALA:HB1	2.01	0.43
4:I:42:LEU:O	4:I:43:ASP:HB2	2.19	0.43
3:A:217:GLU:CD	3:A:599:ARG:HH22	2.22	0.43
3:A:621:ILE:HD11	3:A:686:PHE:CZ	2.54	0.43
3:A:633:LEU:HD22	3:A:638:LEU:HD12	2.00	0.43
3:A:223:LEU:O	3:A:226:LYS:HB3	2.19	0.43
3:F:297:ILE:HG22	3:F:297:ILE:O	2.19	0.43
3:F:321:VAL:HG22	4:I:90:LYS:CE	2.47	0.43
3:A:15:VAL:HG22	3:A:72:LEU:HD21	2.00	0.43
3:A:173:GLN:O	3:A:177:VAL:HG23	2.19	0.43
3:F:551:LEU:HD12	3:F:551:LEU:HA	1.84	0.43
4:I:45:ILE:CD1	4:I:99:LEU:HD13	2.49	0.42
4:I:99:LEU:O	4:I:103:LEU:HG	2.19	0.42
3:A:72:LEU:HA	3:A:75:LEU:CD1	2.46	0.42
3:F:182:LEU:O	3:F:186:LEU:HG	2.19	0.42
3:A:685:ASN:HB3	5:A:5046:HOH:O	2.19	0.42
4:I:58:LEU:HD11	4:I:63:ASN:CG	2.38	0.42
1:X:920:DC:H2"	1:X:921:DA:H5"	1.96	0.42
3:F:17:LYS:HA	3:F:76:GLN:NE2	2.34	0.42
4:I:54:THR:O	4:I:54:THR:HG22	2.19	0.42
3:A:184:LYS:O	3:A:184:LYS:HD3	2.20	0.42
3:F:213:ALA:HA	3:F:597:ASP:OD2	2.19	0.42
2:Z:974:DT:H2"	2:Z:975:DC:C6	2.55	0.42
3:F:556:LEU:HD11	3:F:566:ARG:HH21	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:182:LEU:O	3:A:186:LEU:HG	2.20	0.42
3:F:475:ASP:N	3:F:475:ASP:OD2	2.52	0.42
3:F:488:MET:HE3	3:F:561:ALA:HB3	2.01	0.42
3:A:446:PRO:O	3:A:447:TYR:HB2	2.19	0.42
3:A:297:ILE:CD1	3:A:297:ILE:N	2.81	0.42
4:I:77:THR:HG22	4:I:79:LEU:HD22	2.02	0.42
1:P:817:DT:C2'	1:P:818:DG:H5'	2.36	0.42
3:F:343:GLN:HG3	3:F:362:PRO:HG3	1.98	0.42
3:F:102:LEU:HD12	3:F:123:HIS:CE1	2.55	0.42
3:A:471:GLN:HB3	3:A:697:GLY:O	2.20	0.42
4:B:8:THR:CG2	4:B:11:SER:H	2.30	0.42
3:F:136:LYS:HG3	3:F:173:GLN:NE2	2.34	0.42
3:F:31:TYR:H	3:F:31:TYR:HD1	1.68	0.42
3:F:237:LYS:O	3:F:241:GLU:HG3	2.19	0.42
4:I:12:PHE:CD1	4:I:13:ASP:N	2.81	0.42
3:F:264:TRP:CD1	3:F:344:LYS:HE2	2.55	0.42
3:A:196:ILE:HD12	3:A:196:ILE:N	2.35	0.42
3:F:702:ILE:C	3:F:704:HIS:H	2.22	0.41
3:F:356:TYR:HD2	3:F:360:GLY:O	2.03	0.41
3:F:285:LYS:HB3	3:F:285:LYS:HZ2	1.85	0.41
3:F:109:LEU:HD13	3:F:131:ARG:HG2	2.02	0.41
3:F:554:LYS:HA	3:F:554:LYS:HD3	1.83	0.41
3:F:621:ILE:HD11	3:F:686:PHE:CZ	2.55	0.41
2:Z:971:DT:H2''	2:Z:972:DT:C7	2.51	0.41
3:A:211:LEU:HD21	3:A:598:GLY:C	2.41	0.41
3:F:591:ARG:HD2	5:F:5316:HOH:O	2.18	0.41
3:F:196:ILE:HD12	3:F:196:ILE:N	2.36	0.41
3:F:254:LEU:O	3:F:258:THR:HG23	2.19	0.41
1:P:807:DC:C2'	1:P:808:DG:C5'	2.95	0.41
2:T:868:DT:H2''	2:T:869:DC:H5'	2.02	0.41
3:F:635:GLU:OE2	3:F:635:GLU:HA	2.20	0.41
3:A:628:LYS:HE2	3:A:679:TRP:CD2	2.56	0.41
3:F:525:ILE:HG23	3:F:526:TYR:N	2.35	0.41
3:A:276:HIS:HA	3:A:277:PRO:HD3	1.94	0.41
3:A:525:ILE:O	3:A:529:LEU:HB2	2.21	0.41
3:F:473:GLY:O	3:F:694:GLY:HA2	2.20	0.41
3:A:290:LYS:HD2	3:A:328:PRO:CG	2.51	0.41
3:F:558:ASN:C	3:F:560:PRO:HD3	2.41	0.41
3:A:490:ARG:HD3	3:A:491:PHE:CZ	2.55	0.41
4:I:49:TYR:HE2	4:I:107:LEU:HD12	1.85	0.41
3:F:391:MET:HE3	3:F:395:ARG:HG3	2.02	0.41
3:A:139:TYR:CE2	3:A:159:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:45:ILE:HG13	4:B:99:LEU:HD12	2.02	0.41
3:F:346:LEU:HD13	3:F:372:VAL:HG11	2.03	0.41
3:A:558:ASN:C	3:A:560:PRO:HD3	2.41	0.41
4:I:79:LEU:N	4:I:79:LEU:HD22	2.36	0.41
2:Z:967:DG:H2'	2:Z:968:DT:H72	2.02	0.41
3:A:193:PRO:HB3	3:A:195:GLU:OE1	2.21	0.41
3:F:343:GLN:O	3:F:347:GLN:HG3	2.21	0.41
3:A:488:MET:HE3	3:A:561:ALA:HB3	2.03	0.41
4:B:48:GLU:OE2	4:B:96:LYS:NZ	2.49	0.41
3:A:590:ARG:HD2	3:A:592:TRP:O	2.21	0.41
4:I:20:ASP:HA	4:I:23:ILE:HG13	2.03	0.41
3:A:168:MET:HG3	3:A:168:MET:O	2.20	0.41
3:F:228:GLU:OE1	3:F:420:VAL:N	2.47	0.40
3:A:551:LEU:HA	3:A:551:LEU:HD12	1.91	0.40
3:F:106:ASP:HA	3:F:109:LEU:HD12	2.03	0.40
3:F:158:MET:HB2	3:F:161:TRP:CZ3	2.56	0.40
3:F:633:LEU:HD22	3:F:638:LEU:CD1	2.47	0.40
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.61	0.40
4:I:10:ASP:CG	4:I:11:SER:N	2.75	0.40
3:A:530:TYR:CD1	3:A:611:ASN:HB2	2.56	0.40
1:X:915:DA:H2''	1:X:916:DG:C5'	2.50	0.40
4:I:98:GLN:HA	4:I:101:GLU:HB3	2.02	0.40
1:X:906:DA:H2	2:Z:972:DT:O2	2.04	0.40
3:F:35:ARG:HB3	3:F:36:PRO:CD	2.50	0.40
3:A:57:VAL:HG21	3:A:182:LEU:HD22	2.03	0.40
3:A:356:TYR:HD2	3:A:360:GLY:O	2.04	0.40
3:A:31:TYR:CD1	3:A:31:TYR:N	2.90	0.40
3:F:411:ALA:HB3	3:F:413:ASP:OD1	2.21	0.40
2:Z:952:DT:C2'	2:Z:952:DT:O2	2.69	0.40
3:F:345:LYS:HA	3:F:345:LYS:HE2	2.02	0.40
3:A:554:LYS:HD3	3:A:554:LYS:HA	1.85	0.40
4:I:24:LEU:HD12	4:I:24:LEU:N	2.37	0.40
1:X:917:DT:C2'	1:X:918:DG:C5'	2.96	0.40
4:B:7:LEU:HB2	4:B:58:LEU:HD13	2.02	0.40
4:I:102:PHE:C	4:I:104:ASP:N	2.75	0.40
3:A:189:LYS:HG3	3:A:194:PRO:CG	2.40	0.40
3:A:274:PHE:HE1	4:B:37:MET:HE2	1.86	0.40
4:B:13:ASP:CG	4:B:17:LEU:HD12	2.42	0.40
3:F:125:LEU:HD23	3:F:125:LEU:HA	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:5072:HOH:O	5:F:5072:HOH:O[3.555]	1.46	0.74

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	702/704 (100%)	657 (94%)	39 (6%)	6 (1%)	25	49
3	F	685/704 (97%)	635 (93%)	43 (6%)	7 (1%)	22	45
4	B	103/108 (95%)	89 (86%)	10 (10%)	4 (4%)	5	6
4	I	101/108 (94%)	71 (70%)	19 (19%)	11 (11%)	1	0
All	All	1591/1624 (98%)	1452 (91%)	111 (7%)	28 (2%)	13	25

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	302	LYS
3	A	310	ARG
4	B	18	LYS
4	B	19	ALA
3	F	114	LYS
4	I	11	SER
4	I	20	ASP
4	I	44	GLU
3	A	308	GLU
3	A	313	CYS
4	B	15	ASP
3	F	116	PRO
3	F	117	GLY
3	F	154	TYR
4	I	87	ALA
3	A	152	GLU
4	I	46	ALA
3	A	156	ASP
4	B	84	GLY
3	F	495	GLU

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Mol	Chain	Res	Type
4	I	13	ASP
4	I	16	VAL
4	I	21	GLY
3	F	653	HIS
4	I	18	LYS
4	I	43	ASP
3	F	296	GLY
4	I	45	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	563/582 (97%)	533 (95%)	30 (5%)	32	58
3	F	559/582 (96%)	528 (94%)	31 (6%)	30	56
4	B	84/87 (97%)	79 (94%)	5 (6%)	27	51
4	I	81/87 (93%)	79 (98%)	2 (2%)	60	86
All	All	1287/1338 (96%)	1219 (95%)	68 (5%)	32	58

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

Mol	Chain	Res	Type
3	A	17	LYS
3	A	62	HIS
3	A	75	LEU
3	A	86	GLU
3	A	125	LEU
3	A	173	GLN
3	A	189	LYS
3	A	232	PHE
3	A	241	GLU
3	A	285	LYS
3	A	343	GLN
3	A	358	ASP
3	A	368	VAL
3	A	379	LYS

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Mol	Chain	Res	Type
3	A	391	MET
3	A	410	VAL
3	A	420	VAL
3	A	423	ASN
3	A	426	VAL
3	A	449	GLU
3	A	501	LEU
3	A	529	LEU
3	A	554	LYS
3	A	567	GLU
3	A	584	GLN
3	A	599	ARG
3	A	624	LEU
3	A	630	GLU
3	A	654	ASP
3	A	686	PHE
4	B	15	ASP
4	B	37	MET
4	B	53	LEU
4	B	73	ARG
4	B	80	LEU
3	F	17	LYS
3	F	62	HIS
3	F	75	LEU
3	F	85	ARG
3	F	86	GLU
3	F	110	LEU
3	F	125	LEU
3	F	136	LYS
3	F	168	MET
3	F	169	ASP
3	F	171	ASN
3	F	181	LEU
3	F	232	PHE
3	F	285	LYS
3	F	315	LEU
3	F	343	GLN
3	F	359	LYS
3	F	391	MET
3	F	493	ASN
3	F	499	GLU
3	F	523	THR

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Mol	Chain	Res	Type
3	F	529	LEU
3	F	551	LEU
3	F	559	THR
3	F	566	ARG
3	F	575	GLU
3	F	584	GLN
3	F	599	ARG
3	F	624	LEU
3	F	630	GLU
3	F	686	PHE
4	I	25	VAL
4	I	49	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	101	ASN
3	A	123	HIS
3	A	150	GLN
3	A	171	ASN
3	A	173	GLN
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	423	ASN
3	A	439	GLN
3	A	520	ASN
3	A	558	ASN
3	A	570	GLN
3	A	584	GLN
3	A	667	GLN
4	B	50	GLN
4	B	83	ASN
3	F	123	HIS
3	F	173	GLN
3	F	276	HIS
3	F	450	GLN
3	F	460	HIS
3	F	493	ASN
3	F	520	ASN
3	F	539	GLN
3	F	570	GLN

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Mol	Chain	Res	Type
3	F	584	GLN
3	F	585	GLN
3	F	615	GLN
3	F	667	GLN
4	I	50	GLN
4	I	63	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
1	2DT	P	822	1,2	18,20,21	0.92	1 (5%)	20,28,31	1.41	2 (10%)
1	2DT	X	922	1,2	18,20,21	0.89	1 (5%)	20,28,31	1.70	2 (10%)

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
1	2DT	P	822	1,2	-	0/5/18/19	0/2/2/2
1	2DT	X	922	1,2	-	0/5/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	822	2DT	C6-C5	-2.38	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	922	2DT	C6-C5	-2.30	1.33	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	922	2DT	C6-N1-C2	-5.24	120.92	122.41
1	P	822	2DT	C6-N1-C2	-4.09	121.24	122.41
1	X	922	2DT	C5-C6-N1	2.52	124.04	121.59
1	P	822	2DT	C5-C6-N1	2.21	123.73	121.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	20/22 (90%)	-0.44	0 100 100	50, 100, 170, 171	0
1	X	21/22 (95%)	-0.31	0 100 100	49, 96, 198, 201	0
2	T	22/26 (84%)	-0.51	0 100 100	49, 90, 145, 153	0
2	Z	25/26 (96%)	-0.25	1 (4%) 36 32	49, 97, 183, 192	0
3	A	704/704 (100%)	-0.02	10 (1%) 72 72	38, 61, 116, 153	0
3	F	689/704 (97%)	-0.04	8 (1%) 75 77	38, 60, 105, 143	0
4	B	105/108 (97%)	0.31	7 (6%) 17 15	50, 93, 113, 116	0
4	I	105/108 (97%)	1.88	31 (29%) 1 1	51, 108, 147, 153	0
All	All	1691/1720 (98%)	0.09	57 (3%) 43 39	38, 64, 135, 201	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	16	VAL	17.7
4	I	84	GLY	11.5
4	I	53	LEU	11.1
4	I	83	ASN	9.6
4	I	87	ALA	9.5
4	I	82	LYS	7.7
4	I	19	ALA	6.9
4	I	102	PHE	6.6
3	F	299	LYS	6.6
4	I	86	VAL	6.4
4	I	22	ALA	6.0
4	I	106	ASN	5.2
4	I	105	ALA	5.1
4	I	18	LYS	4.8
4	I	94	LEU	4.7
4	I	17	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
4	I	23	ILE	4.4
4	I	104	ASP	4.3
3	A	318	ARG	4.1
4	I	107	LEU	4.0
3	F	297	ILE	3.9
4	I	85	GLU	3.7
3	A	301	PRO	3.7
4	I	80	LEU	3.6
4	I	21	GLY	3.5
4	I	24	LEU	3.5
4	B	22	ALA	3.4
4	B	16	VAL	3.4
4	I	20	ASP	3.3
4	B	80	LEU	3.3
3	A	324	ALA	3.3
4	I	6	HIS	3.2
3	A	298	PHE	3.2
4	I	3	LYS	3.1
4	I	79	LEU	3.1
3	F	530	TYR	3.0
4	I	4	ILE	3.0
3	F	136	LYS	3.0
4	I	101	GLU	3.0
2	Z	976	DG	2.9
3	A	300	LYS	2.9
3	A	319	GLU	2.8
4	I	9	ASP	2.6
4	B	94	LEU	2.5
4	I	26	ASP	2.5
4	B	102	PHE	2.5
3	A	299	LYS	2.5
4	B	4	ILE	2.4
3	F	318	ARG	2.4
3	F	161	TRP	2.3
3	A	294	VAL	2.2
3	F	296	GLY	2.1
3	A	182	LEU	2.1
4	I	99	LEU	2.1
3	F	315	LEU	2.0
4	B	53	LEU	2.0
3	A	346	LEU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	2DT	P	822	19/20	0.14	-0.76	48,50,55,56	0
1	2DT	X	922	19/20	0.14	-0.93	48,52,57,59	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.