



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 AM UTC

PDB ID : 3L8B / pdb_00003l8b
Title : Crystal structure of a replicative DNA polymerase bound to the oxidized guanine lesion guanidinohydantoin
Authors : Aller, P.; Ye, Y.; Wallace, S.S.; Burrows, C.J.; Doublié, S.
Deposited on : 2009-12-30
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

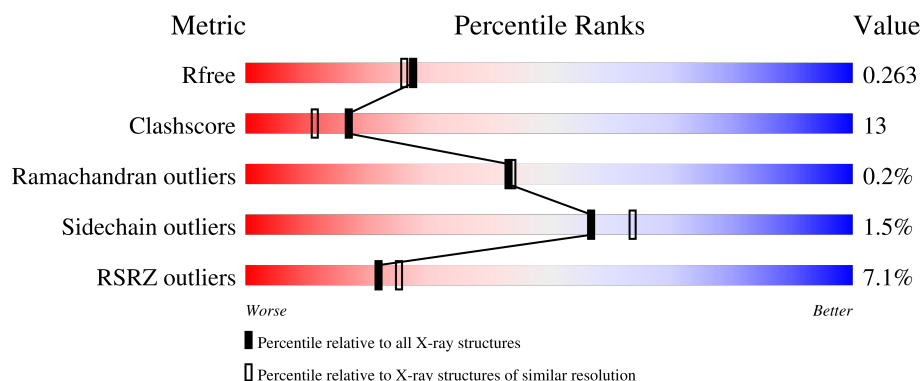
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	906	5% 73% 24% ..
1	B	906	9% 76% 22% ..
2	C	18	22% 44% 17% 6% 11%
2	E	18	6% 17% 50% 17% 6% 11%
3	D	13	15% 15% 77% 8%

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Mol	Chain	Length	Quality of chain
3	F	13	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '15%', a green segment in the middle labeled '23%', and a yellow segment at the end labeled '77%'. The segments are stacked horizontally, with the red segment starting from the left, followed by the green segment, and then the yellow segment.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16717 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 protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	896	Total	C	N	O	S	0	0	0
			7270	4671	1205	1362	32			
1	B	896	Total	C	N	O	S	0	0	0
			7257	4660	1203	1362	32			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
A	904	HIS	-	expression tag	UNP Q38087
A	905	HIS	-	expression tag	UNP Q38087
A	906	HIS	-	expression tag	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
B	904	HIS	-	expression tag	UNP Q38087
B	905	HIS	-	expression tag	UNP Q38087
B	906	HIS	-	expression tag	UNP Q38087

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*C*TP*(G35)P*TP*TP*AP*AP*GP*C P*AP*GP*TP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	P	0	0	0
			326	155	60	96	15			
2	E	16	Total	C	N	O	P	0	0	0
			326	155	60	96	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			265	127	50	76	12			
3	F	13	Total	C	N	O	P	0	0	0
			265	127	50	76	12			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

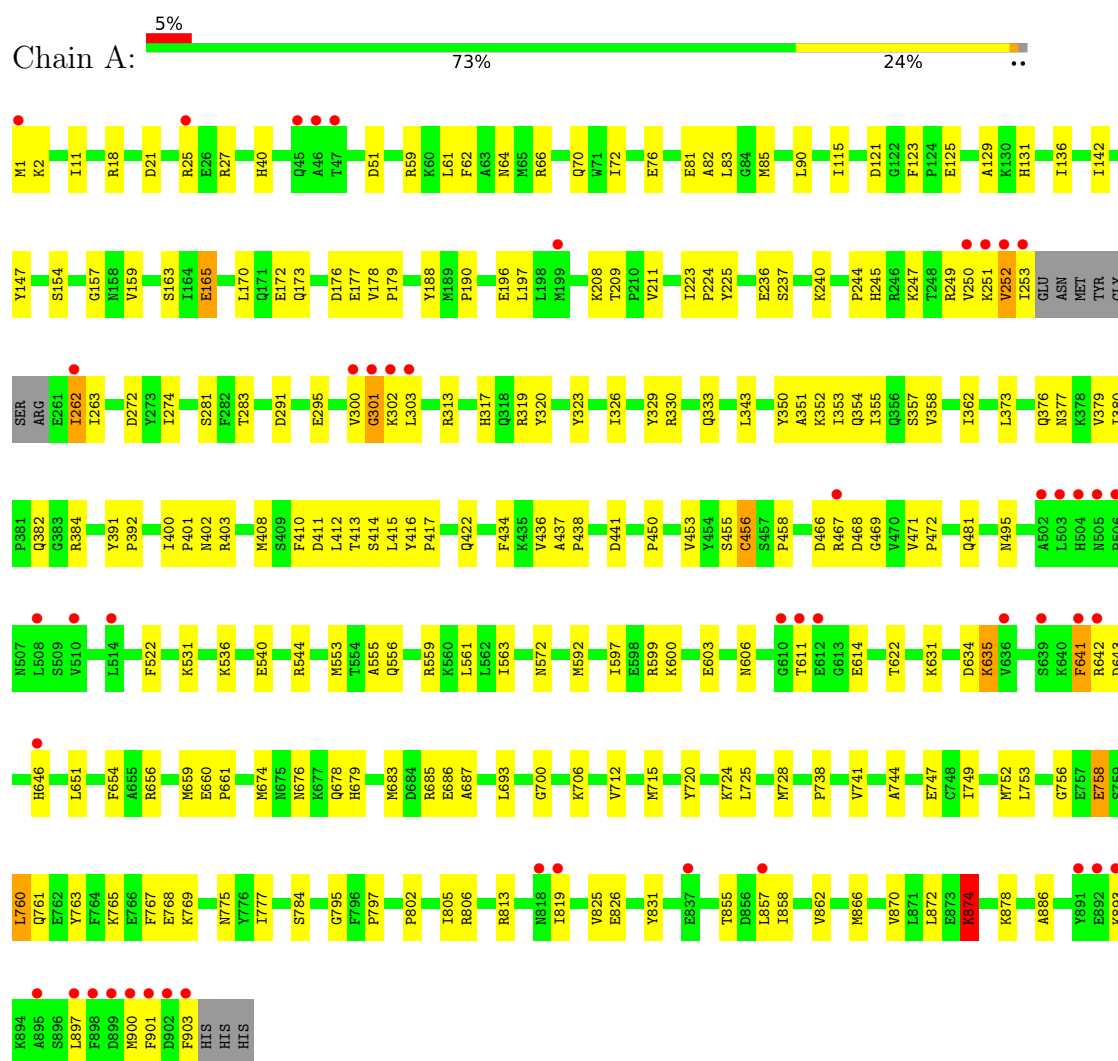
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	462	Total	O	0	0
			462	462		
5	B	428	Total	O	0	0
			428	428		
5	C	27	Total	O	0	0
			27	27		
5	D	19	Total	O	0	0
			19	19		
5	E	39	Total	O	0	0
			39	39		
5	F	23	Total	O	0	0
			23	23		

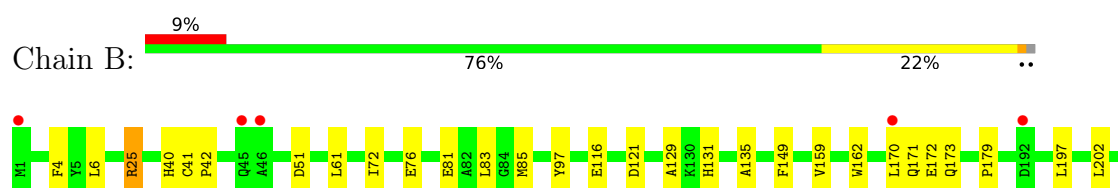
3 Residue-property plots

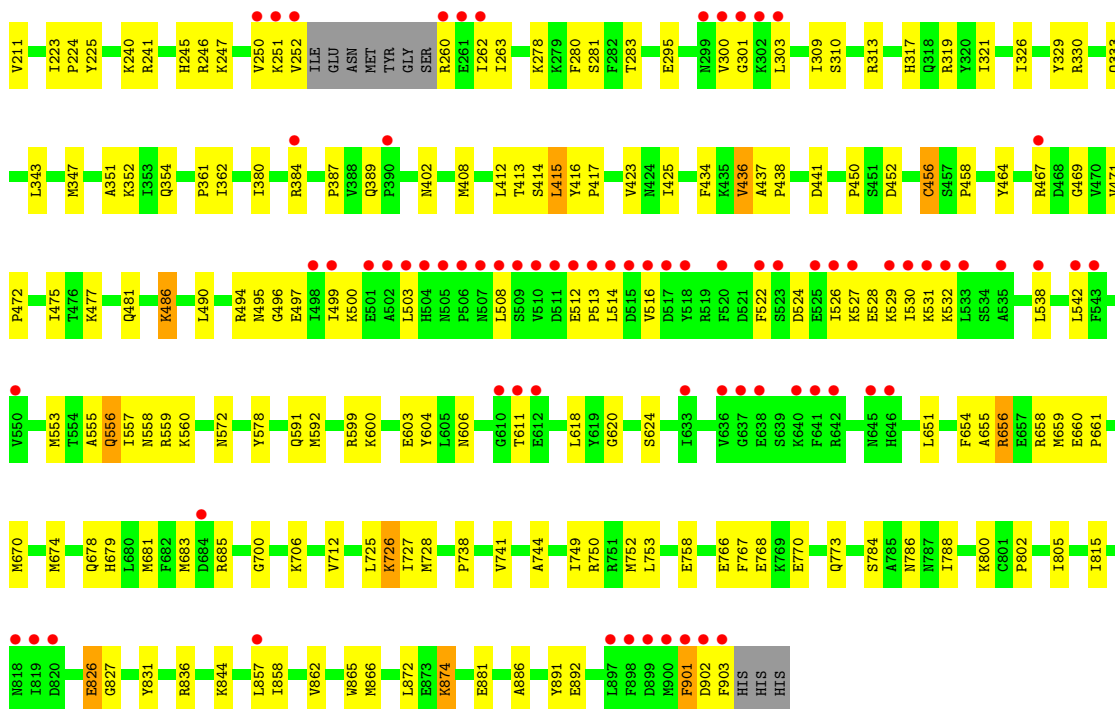
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase



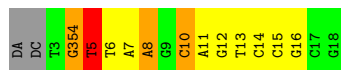
• Molecule 1: DNA polymerase





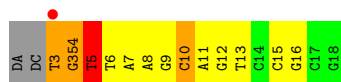
• Molecule 2: DNA (5'-D(*AP*C*TP*(G35)P*TP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3')

Chain C: 22% 44% 17% 6% 11%



• Molecule 2: DNA (5'-D(*AP*C*TP*(G35)P*TP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3')

Chain E: 6% 17% 50% 17% 6% 11%



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

Chain D: 15% 15% 77% 8%



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

Chain F: 15% 23% 77%

C101	
C102	
G103	
G104	
A105	
C106	
T107	
G108	
T111	
A112	
A113	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.28Å 120.25Å 136.96Å 90.00° 95.96° 90.00°	Depositor
Resolution (Å)	48.81 – 2.15 48.81 – 2.15	Depositor EDS
% Data completeness (in resolution range)	88.8 (48.81-2.15) 88.9 (48.81-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.14Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.219 , 0.255 0.228 , 0.263	Depositor DCC
R_{free} test set	25471 reflections (9.44%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16717	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4061e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G35, SO4

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	0.41	0/7449	0.87	14/10077 (0.1%)
1	B	0.40	0/7435	0.87	14/10062 (0.1%)
2	C	0.37	0/339	0.88	3/519 (0.6%)
2	E	0.39	0/339	0.96	3/519 (0.6%)
3	D	0.33	0/297	0.84	1/457 (0.2%)
3	F	0.32	0/297	0.77	1/457 (0.2%)
All	All	0.40	0/16156	0.87	36/22091 (0.2%)

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
2	C	0	2
2	E	0	1
All	All	0	3

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	N-CA-C	-10.08	102.09	111.67
1	B	211	VAL	N-CA-C	-9.10	103.03	111.67
1	B	456	CYS	N-CA-C	7.40	121.13	109.81
1	A	712	VAL	N-CA-C	7.09	118.79	108.58
1	A	456	CYS	N-CA-C	6.57	120.23	109.85
3	F	113	DA	C2'-C3'-O3'	-6.26	102.11	111.50
1	B	354	GLN	N-CA-C	-6.02	100.94	109.96
1	B	712	VAL	N-CA-C	5.90	117.26	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	844	LYS	N-CA-C	5.86	120.05	113.01
1	A	178	VAL	N-CA-C	-5.84	103.23	108.95
1	A	756	GLY	N-CA-C	5.82	118.83	111.85
1	A	354	GLN	N-CA-C	-5.71	101.95	110.23
1	B	436	VAL	N-CA-C	5.60	117.38	108.87
1	A	874	LYS	N-CA-C	5.58	117.44	111.36
1	B	831	TYR	N-CA-C	-5.56	101.47	110.32
1	B	280	PHE	N-CA-C	5.49	120.86	113.72
2	C	13	DT	C5'-C4'-C3'	-5.45	106.72	114.90
1	A	784	SER	N-CA-C	-5.42	102.86	110.50
3	D	103	DG	C2'-C3'-O3'	5.40	119.60	111.50
1	A	400	ILE	N-CA-C	-5.34	102.36	107.76
1	B	6	LEU	N-CA-C	-5.33	105.90	112.72
2	C	10	DC	C5'-C4'-C3'	-5.31	106.94	114.90
1	B	415	LEU	N-CA-C	5.30	120.07	111.37
1	B	452	ASP	N-CA-C	-5.26	106.44	112.92
1	A	403	ARG	N-CA-C	-5.23	102.00	110.32
1	B	874	LYS	N-CA-C	5.23	116.78	111.14
1	A	831	TYR	N-CA-C	-5.22	102.01	110.32
1	A	18	ARG	N-CA-C	-5.18	100.72	109.07
2	E	10	DC	C5'-C4'-C3'	-5.18	107.13	114.90
1	B	784	SER	N-CA-C	-5.14	102.87	110.48
1	A	825	VAL	N-CA-C	5.13	115.70	108.36
2	E	5	DT	N1-C1'-C2'	-5.12	105.81	113.50
2	C	5	DT	N1-C1'-C2'	-5.11	105.83	113.50
1	B	656	ARG	N-CA-C	5.07	116.89	111.36
2	E	3	DT	C2'-C3'-O3'	5.04	119.06	111.50
1	A	641	PHE	N-CA-C	5.01	116.91	109.25

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	5	DT	Sidechain
2	C	8	DA	Sidechain
2	E	5	DT	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7270	0	7105	165	0
1	B	7257	0	7081	164	0
2	C	326	0	183	17	0
2	E	326	0	183	23	0
3	D	265	0	148	17	0
3	F	265	0	148	10	0
4	B	10	0	0	0	0
5	A	462	0	0	18	0
5	B	428	0	0	14	0
5	C	27	0	0	1	0
5	D	19	0	0	0	0
5	E	39	0	0	1	0
5	F	23	0	0	1	0
All	All	16717	0	14848	387	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 13.

All (387) 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:D:103:DG:H2''	3:D:104:DG:O5'	1.65	0.96
2:C:11:DA:H2''	2:C:12:DG:H5'	1.50	0.94
1:A:330:ARG:HH11	1:A:333:GLN:HE22	1.20	0.90
1:A:495:ASN:HD21	1:A:522:PHE:H	1.17	0.88
1:B:726:LYS:HD3	1:B:728:MET:HE3	1.56	0.85
1:A:196:GLU:HG3	5:A:1314:HOH:O	1.76	0.85
2:C:11:DA:H2''	2:C:12:DG:C5'	2.08	0.84
1:B:857:LEU:HD12	1:B:858:ILE:HG23	1.60	0.84
1:B:655:ALA:O	1:B:660:GLU:HG2	1.82	0.79
2:C:7:DA:H2''	2:C:8:DA:H5'	1.63	0.79
1:B:727:ILE:O	1:B:728:MET:HE2	1.83	0.78
3:D:108:DG:H2''	3:D:109:DC:H5'	1.65	0.78
3:D:109:DC:H2''	3:D:110:DT:H5'	1.65	0.78
1:A:303:LEU:HD22	1:A:303:LEU:H	1.49	0.77
1:B:874:LYS:HD2	2:E:12:DG:OP1	1.85	0.77
1:B:347:MET:CA	1:B:558:ASN:HD21	1.99	0.76
2:E:7:DA:H2''	2:E:8:DA:H5''	1.68	0.75
3:F:104:DG:H2''	3:F:105:DA:H5'	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ARG:HD3	5:B:1120:HOH:O	1.87	0.74
1:A:170:LEU:HD23	1:A:173:GLN:NE2	2.03	0.74
1:B:481:GLN:HE21	1:B:559:ARG:HE	1.36	0.74
1:A:330:ARG:HH11	1:A:333:GLN:NE2	1.86	0.73
1:B:330:ARG:HH11	1:B:333:GLN:HE22	1.36	0.73
1:B:656:ARG:HA	1:B:660:GLU:HG3	1.70	0.73
1:B:749:ILE:HA	1:B:752:MET:HE3	1.71	0.73
3:D:108:DG:H2''	3:D:109:DC:C5'	2.20	0.72
1:A:250:VAL:HG22	1:A:263:ILE:HD12	1.72	0.71
1:B:495:ASN:HD21	1:B:522:PHE:H	1.36	0.71
3:F:107:DT:H2''	3:F:108:DG:H5'	1.71	0.71
3:D:107:DT:H2''	3:D:108:DG:H5'	1.71	0.71
1:A:330:ARG:NH1	1:A:333:GLN:HE22	1.87	0.70
3:D:102:DC:H2''	3:D:103:DG:OP2	1.89	0.70
1:A:72:ILE:O	1:A:76:GLU:HG3	1.89	0.70
2:C:4:G35:N12	2:C:4:G35:C5	2.53	0.70
2:E:11:DA:H2''	2:E:12:DG:H5''	1.73	0.70
1:B:758:GLU:HB3	5:B:1143:HOH:O	1.92	0.69
1:B:481:GLN:NE2	1:B:559:ARG:HE	1.90	0.69
1:B:512:GLU:HB3	1:B:513:PRO:HD2	1.74	0.69
1:A:768:GLU:HG3	1:A:872:LEU:HD21	1.75	0.69
3:F:102:DC:H2''	3:F:103:DG:OP2	1.93	0.69
1:A:897:LEU:O	1:A:900:MET:HG2	1.93	0.69
1:B:592:MET:HE1	1:B:674:MET:HE3	1.75	0.68
1:A:249:ARG:HD2	5:A:1069:HOH:O	1.94	0.68
1:B:40:HIS:HD2	5:B:1210:HOH:O	1.76	0.68
1:A:685:ARG:HD3	5:A:967:HOH:O	1.94	0.68
1:A:642:ARG:H	1:A:646:HIS:HD2	1.42	0.67
2:C:11:DA:H1'	2:C:12:DG:H5''	1.74	0.67
3:D:103:DG:C2'	3:D:104:DG:O5'	2.41	0.67
2:E:8:DA:H2''	2:E:9:DG:C8	2.30	0.67
1:B:25:ARG:HH11	1:B:25:ARG:HB3	1.60	0.67
1:A:188:TYR:CE2	1:A:190:PRO:HG3	2.31	0.66
3:F:111:DT:H2''	3:F:112:DA:H5'	1.77	0.66
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.77	0.66
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.76	0.65
1:B:660:GLU:HB2	1:B:661:PRO:HD3	1.79	0.65
1:A:251:LYS:CB	1:A:262:ILE:HG23	2.27	0.65
1:B:303:LEU:HD11	1:B:326:ILE:HG21	1.79	0.65
1:B:654:PHE:HD1	1:B:659:MET:HE2	1.61	0.64
1:A:728:MET:HE2	3:D:113:DA:OP2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:CYS:O	1:A:674:MET:HG3	1.97	0.64
2:E:11:DA:H2''	2:E:12:DG:C5'	2.27	0.63
1:A:700:GLY:HA2	1:A:753:LEU:HD22	1.78	0.63
1:A:758:GLU:HG2	5:A:945:HOH:O	1.96	0.63
1:A:654:PHE:CD1	1:A:659:MET:HE2	2.34	0.63
1:B:901:PHE:HD2	1:B:901:PHE:N	1.97	0.63
1:B:72:ILE:O	1:B:76:GLU:HG3	1.99	0.63
1:B:815:ILE:HG22	1:B:857:LEU:HD11	1.80	0.62
2:E:8:DA:H2''	2:E:9:DG:H8	1.64	0.62
1:B:655:ALA:HA	1:B:659:MET:HE3	1.81	0.62
1:B:387:PRO:HG2	1:B:389:GLN:HE21	1.64	0.62
3:D:111:DT:H2''	3:D:112:DA:H5'	1.82	0.61
1:B:700:GLY:HA2	1:B:753:LEU:HD22	1.81	0.61
1:B:171:GLN:HE22	1:B:319:ARG:HH12	1.48	0.61
3:F:107:DT:H2''	3:F:108:DG:C5'	2.31	0.61
1:B:836:ARG:NH1	1:B:865:TRP:HA	2.16	0.61
3:D:109:DC:H2''	3:D:110:DT:C5'	2.29	0.61
3:F:104:DG:H2''	3:F:105:DA:C5'	2.30	0.61
1:A:654:PHE:HD1	1:A:659:MET:HE2	1.66	0.60
3:D:108:DG:H1'	3:D:109:DC:H5''	1.83	0.60
1:B:300:VAL:HG23	1:B:300:VAL:O	2.01	0.60
1:A:450:PRO:HG2	5:A:1115:HOH:O	2.02	0.60
1:B:408:MET:HE2	1:B:651:LEU:HB3	1.83	0.60
1:A:466:ASP:OD2	1:A:467:ARG:HG2	2.02	0.60
1:B:303:LEU:N	1:B:303:LEU:HD22	2.17	0.59
2:C:11:DA:C2'	2:C:12:DG:C5'	2.79	0.59
2:E:3:DT:H2''	2:E:4:G35:OP1	2.01	0.59
1:B:456:CYS:O	1:B:674:MET:HG3	2.03	0.59
1:A:362:ILE:HD11	1:A:572:ASN:CG	2.28	0.59
1:A:614:GLU:CD	1:A:631:LYS:HE3	2.28	0.59
1:B:901:PHE:O	1:B:902:ASP:HB2	2.02	0.59
1:A:481:GLN:HE21	1:A:559:ARG:HE	1.50	0.59
3:F:105:DA:H2''	3:F:106:DC:O5'	2.03	0.58
1:A:481:GLN:NE2	1:A:559:ARG:HE	2.01	0.58
1:B:901:PHE:N	1:B:901:PHE:CD2	2.69	0.58
1:A:170:LEU:HD23	1:A:173:GLN:HE21	1.68	0.58
1:B:347:MET:HA	1:B:558:ASN:HD21	1.67	0.58
1:B:471:VAL:HB	1:B:472:PRO:HD3	1.86	0.58
1:A:179:PRO:HG2	1:A:329:TYR:CE2	2.38	0.58
1:B:361:PRO:HD2	2:E:4:G35:O5'	2.04	0.57
1:B:362:ILE:HG13	2:E:4:G35:H5'A	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD12	1:A:357:SER:HB2	1.86	0.57
2:E:10:DC:H2''	2:E:11:DA:H5'	1.85	0.57
1:A:413:THR:O	1:A:414:SER:C	2.46	0.57
1:B:83:LEU:N	1:B:83:LEU:HD12	2.20	0.57
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.85	0.57
1:A:11:ILE:HD13	1:A:247:LYS:HG3	1.85	0.57
1:B:508:LEU:HD12	1:B:508:LEU:N	2.20	0.57
2:C:11:DA:C2'	2:C:12:DG:H5''	2.35	0.57
1:B:727:ILE:C	1:B:728:MET:HE2	2.30	0.57
1:A:165:GLU:CD	1:A:165:GLU:H	2.12	0.56
1:B:836:ARG:HH12	1:B:865:TRP:HA	1.70	0.56
1:B:499:ILE:HG21	1:B:542:LEU:HB2	1.88	0.56
1:A:121:ASP:OD1	1:A:131:HIS:HE1	1.88	0.56
1:A:495:ASN:HD21	1:A:522:PHE:N	1.98	0.56
1:B:874:LYS:HD2	2:E:12:DG:P	2.45	0.56
1:A:157:GLY:O	1:A:313:ARG:NH2	2.39	0.56
1:A:422:GLN:HG3	1:A:678:GLN:O	2.05	0.56
1:A:553:MET:O	1:A:556:GLN:HG3	2.06	0.56
1:A:300:VAL:O	1:A:300:VAL:HG23	2.05	0.55
1:A:163:SER:OG	1:A:165:GLU:HG2	2.06	0.55
1:A:458:PRO:HG3	1:A:592:MET:SD	2.47	0.55
1:B:881:GLU:HG2	1:B:891:TYR:HE1	1.71	0.55
1:A:412:LEU:HG	1:A:683:MET:HE3	1.89	0.55
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.87	0.55
2:C:11:DA:C1'	2:C:12:DG:H5''	2.36	0.55
1:B:654:PHE:CD1	1:B:659:MET:HE2	2.40	0.55
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.89	0.55
2:C:14:DC:H2''	2:C:15:DC:C5'	2.37	0.55
1:A:303:LEU:HD11	1:A:326:ILE:HG21	1.88	0.55
1:B:408:MET:HE2	1:B:651:LEU:HD22	1.88	0.55
1:B:529:LYS:HA	1:B:532:LYS:HE2	1.89	0.55
1:A:411:ASP:CG	1:A:686:GLU:HG3	2.33	0.54
1:B:245:HIS:O	1:B:247:LYS:HG2	2.07	0.54
1:B:387:PRO:HG2	1:B:389:GLN:NE2	2.22	0.54
1:A:434:PHE:CE2	1:A:450:PRO:HB3	2.43	0.54
1:A:295:GLU:OE2	1:A:301:GLY:HA2	2.06	0.54
1:A:40:HIS:HE1	1:A:51:ASP:OD2	1.91	0.54
1:A:540:GLU:O	1:A:544:ARG:HG3	2.08	0.54
1:B:362:ILE:HD11	1:B:572:ASN:CG	2.33	0.54
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.43	0.54
1:B:555:ALA:O	1:B:559:ARG:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ARG:HA	1:B:660:GLU:CG	2.37	0.54
1:A:40:HIS:HD2	5:A:1075:HOH:O	1.90	0.53
1:A:272:ASP:OD1	1:A:274:ILE:HG22	2.07	0.53
1:A:857:LEU:CD1	1:A:858:ILE:HG23	2.37	0.53
1:B:412:LEU:HD13	1:B:415:LEU:HD13	1.89	0.53
1:A:350:TYR:OH	1:A:481:GLN:NE2	2.39	0.53
1:B:592:MET:CE	1:B:674:MET:HE3	2.38	0.53
1:B:362:ILE:HD11	1:B:572:ASN:HB3	1.91	0.53
1:A:61:LEU:HD13	1:A:61:LEU:C	2.34	0.53
1:A:555:ALA:O	1:A:559:ARG:HG2	2.09	0.53
1:A:303:LEU:H	1:A:303:LEU:CD2	2.21	0.53
1:A:606:ASN:OD1	1:A:611:THR:HG23	2.08	0.53
1:B:347:MET:CB	1:B:558:ASN:HD21	2.22	0.52
1:B:862:VAL:O	1:B:866:MET:HG3	2.08	0.52
1:A:878:LYS:HD3	5:C:55:HOH:O	2.10	0.52
2:C:14:DC:H2''	2:C:15:DC:H5''	1.90	0.52
2:E:11:DA:H5'	2:E:11:DA:C8	2.44	0.52
1:B:171:GLN:HE22	1:B:319:ARG:NH1	2.08	0.52
2:E:11:DA:H5'	2:E:11:DA:H8	1.73	0.52
1:A:66:ARG:O	1:A:70:GLN:HG2	2.09	0.52
1:A:797:PRO:HG3	1:A:806:ARG:NH1	2.24	0.52
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.44	0.52
1:A:802:PRO:HB2	1:A:805:ILE:HG12	1.91	0.52
1:B:413:THR:O	1:B:414:SER:C	2.52	0.52
2:E:7:DA:H2''	2:E:8:DA:C5'	2.39	0.52
1:A:303:LEU:HD22	1:A:303:LEU:N	2.20	0.52
1:A:25:ARG:HD2	1:A:27:ARG:NH2	2.24	0.52
1:B:303:LEU:HD22	1:B:303:LEU:H	1.75	0.52
1:A:600:LYS:HE2	5:A:1211:HOH:O	2.09	0.51
1:A:402:ASN:HA	1:A:886:ALA:O	2.10	0.51
1:B:179:PRO:HG2	1:B:329:TYR:CE2	2.45	0.51
1:B:241:ARG:HA	1:B:246:ARG:HD3	1.93	0.51
1:A:147:TYR:OH	1:A:208:LYS:NZ	2.44	0.51
2:E:12:DG:H1'	5:E:959:HOH:O	2.11	0.51
1:A:656:ARG:HA	1:A:660:GLU:HG3	1.91	0.51
1:A:720:TYR:CZ	1:A:724:LYS:NZ	2.79	0.51
1:B:529:LYS:HA	1:B:532:LYS:CE	2.40	0.51
1:B:171:GLN:HE22	1:B:319:ARG:HH22	1.57	0.51
1:B:281:SER:O	1:B:283:THR:HG23	2.11	0.51
1:B:458:PRO:HG3	1:B:592:MET:SD	2.50	0.51
1:A:172:GLU:HB2	5:A:1207:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD12	1:B:83:LEU:H	1.76	0.51
1:B:526:ILE:O	1:B:530:ILE:HG13	2.11	0.51
1:B:768:GLU:HG3	1:B:872:LEU:HD21	1.92	0.51
1:A:775:ASN:OD1	1:A:777:ILE:HB	2.11	0.50
1:B:171:GLN:NE2	1:B:319:ARG:HH22	2.08	0.50
1:A:209:THR:HG21	1:A:244:PRO:HB3	1.94	0.50
1:A:687:ALA:HB2	1:A:715:MET:HE1	1.93	0.50
1:B:679:HIS:HD2	5:B:1008:HOH:O	1.94	0.50
1:A:250:VAL:HG22	1:A:263:ILE:CD1	2.40	0.50
1:B:464:TYR:HB3	1:B:467:ARG:HH11	1.76	0.50
1:B:556:GLN:HG3	1:B:557:ILE:N	2.26	0.50
1:B:81:GLU:HG2	1:B:83:LEU:CD1	2.41	0.49
1:B:412:LEU:HG	1:B:683:MET:HE3	1.93	0.49
1:B:436:VAL:HG22	1:B:437:ALA:O	2.12	0.49
1:B:494:ARG:O	1:B:497:GLU:HB2	2.12	0.49
1:B:250:VAL:HG22	1:B:263:ILE:HD12	1.93	0.49
1:B:592:MET:SD	1:B:674:MET:HE3	2.52	0.49
1:A:123:PHE:HD2	1:A:125:GLU:OE2	1.96	0.49
1:B:438:PRO:HD2	1:B:441:ASP:OD2	2.13	0.49
3:D:106:DC:H2''	3:D:107:DT:OP2	2.12	0.49
3:D:107:DT:H2''	3:D:108:DG:C5'	2.42	0.49
1:B:40:HIS:HE1	1:B:51:ASP:OD2	1.96	0.49
1:B:4:PHE:HA	1:B:97:TYR:CE2	2.48	0.48
1:B:81:GLU:HB2	1:B:384:ARG:NH2	2.28	0.48
1:B:252:VAL:O	1:B:260:ARG:O	2.31	0.48
1:B:295:GLU:OE2	1:B:301:GLY:HA2	2.13	0.48
1:B:384:ARG:HD3	5:B:938:HOH:O	2.12	0.48
1:A:795:GLY:O	1:A:813:ARG:HD3	2.13	0.48
1:A:819:ILE:HG22	5:A:1205:HOH:O	2.12	0.48
1:A:410:PHE:HB3	1:A:683:MET:HG2	1.96	0.48
1:A:64:ASN:OD1	1:A:66:ARG:HB3	2.13	0.48
2:E:5:DT:H2'	2:E:6:DT:H72	1.95	0.48
1:A:765:LYS:HG2	1:A:769:LYS:HE2	1.94	0.48
2:E:15:DC:H2''	2:E:16:DG:C8	2.48	0.48
1:A:170:LEU:HD12	1:A:177:GLU:CD	2.38	0.48
1:A:724:LYS:NZ	1:A:724:LYS:HB2	2.28	0.48
1:A:66:ARG:HH21	1:A:70:GLN:NE2	2.12	0.48
1:A:142:ILE:HA	5:A:1286:HOH:O	2.13	0.48
1:A:411:ASP:OD1	1:A:686:GLU:HG3	2.13	0.48
1:B:516:VAL:HG11	1:B:526:ILE:HD12	1.95	0.48
1:A:172:GLU:H	1:A:172:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:PHE:HB2	1:A:903:PHE:CE2	2.48	0.48
2:C:7:DA:H2''	2:C:8:DA:C5'	2.38	0.48
1:A:176:ASP:HA	1:A:319:ARG:NH2	2.29	0.48
1:A:252:VAL:O	1:A:253:ILE:C	2.56	0.47
1:B:25:ARG:HB3	1:B:25:ARG:NH1	2.27	0.47
1:B:351:ALA:O	1:B:352:LYS:HB2	2.14	0.47
1:B:251:LYS:CB	1:B:262:ILE:HG23	2.44	0.47
1:A:237:SER:HB3	5:A:986:HOH:O	2.14	0.47
1:B:553:MET:O	1:B:556:GLN:HG3	2.15	0.47
1:A:862:VAL:O	1:A:866:MET:HG3	2.14	0.47
1:B:343:LEU:C	1:B:343:LEU:HD23	2.39	0.47
1:B:450:PRO:HG2	5:B:1118:HOH:O	2.14	0.47
1:B:499:ILE:CG2	1:B:542:LEU:HB2	2.45	0.47
2:C:14:DC:C2'	2:C:15:DC:H5''	2.44	0.47
1:A:1:MET:HB2	5:A:1345:HOH:O	2.14	0.47
2:C:5:DT:H2'	2:C:6:DT:H72	1.97	0.47
3:D:111:DT:H2''	3:D:112:DA:C5'	2.44	0.47
1:B:524:ASP:O	1:B:528:GLU:HG2	2.15	0.46
1:A:495:ASN:ND2	1:A:522:PHE:H	1.99	0.46
1:B:170:LEU:N	1:B:170:LEU:HD22	2.30	0.46
1:B:250:VAL:HG22	1:B:263:ILE:CD1	2.45	0.46
1:B:408:MET:CE	1:B:651:LEU:HD22	2.46	0.46
1:B:706:LYS:HE3	2:E:7:DA:N3	2.31	0.46
1:B:171:GLN:HE22	1:B:319:ARG:NH2	2.14	0.46
1:A:870:VAL:HG12	1:A:874:LYS:HE3	1.96	0.46
1:B:681:MET:HE2	1:B:681:MET:HA	1.97	0.46
1:A:760:LEU:C	1:A:760:LEU:HD13	2.40	0.46
1:B:434:PHE:CE2	1:B:450:PRO:HB3	2.50	0.46
1:A:59:ARG:NH2	1:A:61:LEU:HD23	2.30	0.46
1:B:197:LEU:C	1:B:197:LEU:HD23	2.41	0.46
1:A:376:GLN:O	1:A:377:ASN:HB2	2.15	0.46
1:A:531:LYS:HB2	5:A:1334:HOH:O	2.16	0.46
1:A:857:LEU:HD13	1:A:858:ILE:HG23	1.97	0.46
1:B:51:ASP:HB2	5:B:999:HOH:O	2.15	0.46
1:B:121:ASP:OD1	1:B:131:HIS:HE1	1.98	0.46
1:A:83:LEU:HD12	1:A:83:LEU:N	2.30	0.45
1:A:455:SER:OG	1:A:676:ASN:HA	2.16	0.45
1:A:466:ASP:OD2	1:A:467:ARG:N	2.49	0.45
1:B:469:GLY:C	1:B:472:PRO:HD2	2.41	0.45
3:F:107:DT:H1'	3:F:108:DG:H5''	1.98	0.45
1:B:606:ASN:HA	1:B:611:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:LEU:HD11	1:B:750:ARG:HB2	1.98	0.45
1:A:870:VAL:CG1	1:A:874:LYS:HE3	2.47	0.45
2:C:15:DC:H2''	2:C:16:DG:C8	2.51	0.45
1:A:634:ASP:O	1:A:635:LYS:C	2.59	0.45
1:B:313:ARG:HD2	5:B:921:HOH:O	2.15	0.45
1:B:362:ILE:HD11	1:B:572:ASN:CB	2.47	0.45
1:A:81:GLU:HB2	1:A:384:ARG:NH2	2.31	0.45
1:A:469:GLY:C	1:A:472:PRO:HD2	2.42	0.45
1:B:788:ILE:HG13	1:B:826:GLU:OE2	2.17	0.45
1:A:61:LEU:HD13	1:A:62:PHE:N	2.31	0.45
2:E:3:DT:C5'	2:E:3:DT:H6	2.29	0.45
1:A:245:HIS:O	1:A:247:LYS:HG2	2.17	0.45
1:B:303:LEU:H	1:B:303:LEU:CD2	2.30	0.45
1:B:467:ARG:HH11	1:B:467:ARG:HG2	1.80	0.45
1:A:83:LEU:HB3	1:A:379:VAL:HG12	1.99	0.45
1:A:408:MET:HE2	1:A:651:LEU:HB3	1.99	0.45
1:A:700:GLY:CA	1:A:753:LEU:HD22	2.44	0.45
1:A:82:ALA:O	1:A:382:GLN:HB2	2.17	0.45
1:A:747:GLU:HG2	1:A:763:TYR:CE2	2.52	0.44
1:B:471:VAL:O	1:B:475:ILE:HG22	2.16	0.44
2:E:12:DG:H2'	2:E:13:DT:H72	2.00	0.44
1:A:51:ASP:HB2	5:A:1366:HOH:O	2.17	0.44
1:A:641:PHE:HA	1:A:646:HIS:CD2	2.52	0.44
1:B:514:LEU:HD23	1:B:526:ILE:HG23	1.99	0.44
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.99	0.44
1:A:855:THR:HG23	1:A:858:ILE:HG12	2.00	0.44
1:A:749:ILE:HA	1:A:752:MET:HE3	1.99	0.44
1:B:162:TRP:CD1	1:B:321:ILE:HB	2.52	0.44
1:B:402:ASN:HA	1:B:886:ALA:O	2.17	0.44
1:B:604:TYR:OH	1:B:658:ARG:HB3	2.17	0.44
3:D:108:DG:C2'	3:D:109:DC:H5''	2.47	0.44
1:A:351:ALA:O	1:A:352:LYS:HB2	2.15	0.44
1:A:436:VAL:HG22	1:A:437:ALA:O	2.18	0.44
1:B:600:LYS:HE2	5:B:1093:HOH:O	2.17	0.44
1:A:129:ALA:HA	1:A:225:TYR:CZ	2.52	0.44
1:B:85:MET:HA	1:B:380:ILE:HD11	2.00	0.44
1:A:320:TYR:O	1:A:323:TYR:HB3	2.17	0.43
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.53	0.43
1:B:172:GLU:HB2	5:B:1272:HOH:O	2.17	0.43
1:A:291:ASP:OD2	1:A:302:LYS:HA	2.18	0.43
1:A:559:ARG:O	1:A:563:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:SER:HA	5:B:1185:HOH:O	2.17	0.43
1:B:766:GLU:O	1:B:770:GLU:HG2	2.19	0.43
1:B:591:GLN:NE2	5:B:1176:HOH:O	2.51	0.43
1:A:2:LYS:HA	1:A:2:LYS:HE2	2.00	0.43
1:A:115:ILE:HG22	1:A:136:ILE:HG12	2.00	0.43
1:A:720:TYR:CD1	1:A:724:LYS:HE3	2.54	0.43
1:B:309:ILE:HG22	5:B:1156:HOH:O	2.18	0.43
1:A:131:HIS:HD2	5:A:1055:HOH:O	2.02	0.43
1:A:281:SER:O	1:A:283:THR:HG23	2.19	0.43
1:B:786:ASN:ND2	1:B:827:GLY:HA2	2.34	0.43
1:B:891:TYR:CD2	1:B:892:GLU:HG3	2.54	0.43
1:A:761:GLN:NE2	1:A:893:LYS:HA	2.34	0.43
1:B:303:LEU:N	1:B:303:LEU:CD2	2.82	0.43
1:B:503:LEU:HD21	1:B:538:LEU:HB2	2.00	0.43
3:D:108:DG:C2'	3:D:109:DC:C5'	2.93	0.43
1:B:278:LYS:NZ	5:B:1334:HOH:O	2.50	0.43
1:B:599:ARG:O	1:B:603:GLU:HG3	2.19	0.43
1:A:614:GLU:CG	1:A:631:LYS:HE3	2.49	0.42
1:A:758:GLU:CD	1:A:758:GLU:H	2.27	0.42
1:A:373:LEU:HD12	1:A:380:ILE:HG22	2.01	0.42
1:B:116:GLU:HB2	1:B:135:ALA:HB3	2.00	0.42
1:B:477:LYS:O	1:B:481:GLN:HG3	2.19	0.42
1:B:802:PRO:HB2	1:B:805:ILE:HG12	2.00	0.42
1:A:643:ASP:HA	1:A:693:LEU:HD23	2.00	0.42
1:B:330:ARG:HH11	1:B:333:GLN:NE2	2.10	0.42
1:B:591:GLN:HE21	1:B:591:GLN:HB3	1.59	0.42
1:B:744:ALA:HB2	1:B:767:PHE:CE2	2.55	0.42
1:A:85:MET:HA	1:A:380:ILE:HD11	2.00	0.42
1:A:599:ARG:O	1:A:603:GLU:HG3	2.20	0.42
1:B:527:LYS:O	1:B:531:LYS:HG3	2.20	0.42
1:A:262:ILE:HD12	5:A:1082:HOH:O	2.19	0.42
1:B:416:TYR:HB2	1:B:417:PRO:HD3	2.02	0.42
1:B:578:TYR:CD1	1:B:578:TYR:C	2.97	0.42
2:E:11:DA:H2''	2:E:12:DG:O5'	2.19	0.42
1:B:496:GLY:O	1:B:500:LYS:HG3	2.19	0.42
1:A:747:GLU:HG2	1:A:763:TYR:CZ	2.55	0.42
2:C:10:DC:H2''	2:C:11:DA:C8	2.55	0.42
1:B:41:CYS:HB2	1:B:42:PRO:HD2	2.02	0.42
1:B:471:VAL:N	1:B:472:PRO:CD	2.83	0.42
1:B:726:LYS:CD	1:B:728:MET:HE3	2.37	0.41
1:A:679:HIS:HD2	5:A:909:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PRO:HG2	2:E:4:G35:C8	2.49	0.41
1:B:362:ILE:HG13	2:E:4:G35:C5'	2.50	0.41
1:B:738:PRO:HG2	1:B:741:VAL:CG2	2.50	0.41
1:A:90:LEU:HD21	1:A:353:ILE:HG22	2.01	0.41
1:A:326:ILE:O	1:A:330:ARG:HG2	2.21	0.41
1:A:401:PRO:O	1:A:402:ASN:HB2	2.19	0.41
1:A:600:LYS:HD3	1:A:600:LYS:HA	1.87	0.41
1:A:738:PRO:HG2	1:A:741:VAL:CG2	2.50	0.41
1:B:620:GLY:HA2	1:B:624:SER:O	2.21	0.41
1:B:902:ASP:O	1:B:903:PHE:C	2.63	0.41
1:A:438:PRO:HD2	1:A:441:ASP:OD2	2.20	0.41
1:A:597:ILE:HD12	1:A:597:ILE:HA	1.94	0.41
1:A:21:ASP:C	1:A:21:ASP:OD1	2.64	0.41
1:A:416:TYR:HB2	1:A:417:PRO:HD3	2.03	0.41
3:D:107:DT:H1'	3:D:108:DG:H5''	2.01	0.41
1:A:179:PRO:HG2	1:A:329:TYR:CD2	2.55	0.41
1:A:857:LEU:HD12	1:A:858:ILE:HG23	2.01	0.41
3:F:105:DA:H1'	5:F:691:HOH:O	2.20	0.41
1:B:240:LYS:O	1:B:246:ARG:HA	2.21	0.41
1:A:236:GLU:HG2	1:A:240:LYS:HE2	2.02	0.41
1:B:343:LEU:CD2	1:B:347:MET:HE3	2.51	0.41
2:C:15:DC:H5'	2:C:15:DC:H6	1.85	0.41
1:A:724:LYS:NZ	1:A:724:LYS:CB	2.84	0.41
1:A:725:LEU:HD22	1:A:753:LEU:HD12	2.03	0.41
1:A:897:LEU:O	1:A:900:MET:CG	2.67	0.41
1:B:170:LEU:HD23	1:B:173:GLN:OE1	2.21	0.41
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.94	0.41
3:F:103:DG:H2''	3:F:104:DG:OP2	2.20	0.41
1:A:197:LEU:HD23	1:A:197:LEU:C	2.45	0.41
1:B:129:ALA:HA	1:B:225:TYR:CZ	2.56	0.41
1:B:423:VAL:HB	1:B:425:ILE:HG13	2.03	0.41
1:A:706:LYS:HE3	2:C:7:DA:N3	2.36	0.40
1:B:472:PRO:HA	1:B:475:ILE:HG22	2.03	0.40
1:A:2:LYS:HB2	5:A:1324:HOH:O	2.21	0.40
1:A:343:LEU:HD21	1:A:561:LEU:HD11	2.03	0.40
1:B:149:PHE:N	1:B:149:PHE:CD1	2.90	0.40
1:B:486:LYS:O	1:B:490:LEU:HD13	2.22	0.40
1:B:800:LYS:HE2	1:B:800:LYS:HB3	1.97	0.40
1:A:170:LEU:HB2	1:A:173:GLN:HE21	1.86	0.40
1:A:355:ILE:O	1:A:358:VAL:HG13	2.21	0.40
1:B:592:MET:HE3	1:B:670:MET:SD	2.61	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	
1	A	892/906 (98%)	864 (97%)	25 (3%)	3 (0%)	36	34
1	B	892/906 (98%)	857 (96%)	35 (4%)	0	100	100
All	All	1784/1812 (98%)	1721 (96%)	60 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	VAL
1	A	301	GLY
1	A	622	THR

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	
1	A	782/803 (97%)	771 (99%)	11 (1%)	59	66
1	B	780/803 (97%)	768 (98%)	12 (2%)	57	64
All	All	1562/1606 (97%)	1539 (98%)	23 (2%)	57	64

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	SER
1	A	165	GLU
1	A	262	ILE
1	A	453	VAL
1	A	468	ASP
1	A	536	LYS
1	A	635	LYS
1	A	758	GLU
1	A	760	LEU
1	A	826	GLU
1	A	874	LYS
1	B	25	ARG
1	B	61	LEU
1	B	202	LEU
1	B	486	LYS
1	B	556	GLN
1	B	560	LYS
1	B	618	LEU
1	B	678	GLN
1	B	726	LYS
1	B	773	GLN
1	B	826	GLU
1	B	901	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	128	GLN
1	A	131	HIS
1	A	173	GLN
1	A	299	ASN
1	A	333	GLN
1	A	342	ASN
1	A	354	GLN
1	A	376	GLN
1	A	386	HIS
1	A	389	GLN
1	A	481	GLN
1	A	495	ASN
1	A	505	ASN
1	A	539	ASN
1	A	546	GLN

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Mol	Chain	Res	Type
1	A	591	GLN
1	A	646	HIS
1	A	679	HIS
1	A	733	GLN
1	A	761	GLN
1	A	773	GLN
1	A	786	ASN
1	A	787	ASN
1	A	818	ASN
1	A	823	GLN
1	B	40	HIS
1	B	112	ASN
1	B	171	GLN
1	B	206	GLN
1	B	333	GLN
1	B	354	GLN
1	B	389	GLN
1	B	459	ASN
1	B	481	GLN
1	B	495	ASN
1	B	507	ASN
1	B	546	GLN
1	B	558	ASN
1	B	591	GLN
1	B	678	GLN
1	B	679	HIS
1	B	733	GLN
1	B	742	GLN
1	B	761	GLN
1	B	786	ASN
1	B	787	ASN
1	B	823	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	G35	E	4	2	18,23,24	1.31	4 (22%)	18,33,36	1.52	1 (5%)
2	G35	C	4	2	18,23,24	1.34	4 (22%)	18,33,36	1.50	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G35	E	4	2	-	1/11/41/42	0/2/2/2
2	G35	C	4	2	-	2/11/41/42	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	G35	C5-N7	-3.25	1.33	1.37
2	E	4	G35	C5-N7	-3.13	1.33	1.37
2	C	4	G35	C8-N9	-2.74	1.33	1.37
2	E	4	G35	C4-N3	2.69	1.47	1.44
2	E	4	G35	C8-N7	-2.60	1.33	1.38
2	E	4	G35	C8-N9	-2.59	1.33	1.37
2	C	4	G35	C4-N3	2.57	1.47	1.44
2	C	4	G35	C8-N7	-2.44	1.33	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	G35	N7-C8-N9	5.73	112.45	107.55
2	E	4	G35	N7-C8-N9	5.55	112.30	107.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	G35	C5-C4-N3-C2
2	E	4	G35	C2'-C1'-N9-C4
2	C	4	G35	N9-C4-N3-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	G35	5	0
2	C	4	G35	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
4	SO4	B	908	-	4,4,4	0.36	0	6,6,6	0.12	0
4	SO4	B	907	-	4,4,4	0.36	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	896/906 (98%)	0.16	47 (5%) 33 36	10, 24, 48, 78	0
1	B	896/906 (98%)	0.34	79 (8%) 15 17	11, 26, 58, 82	0
2	C	15/18 (83%)	-0.04	0 100 100	20, 28, 42, 44	0
2	E	15/18 (83%)	0.19	1 (6%) 24 27	21, 27, 44, 56	0
3	D	13/13 (100%)	0.53	2 (15%) 5 5	21, 25, 79, 84	0
3	F	13/13 (100%)	0.50	2 (15%) 5 5	22, 24, 85, 89	0
All	All	1848/1874 (98%)	0.25	131 (7%) 22 25	10, 25, 54, 89	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	903	PHE	6.9
1	A	252	VAL	6.9
1	A	253	ILE	6.3
1	B	252	VAL	6.2
1	B	901	PHE	5.9
1	B	510	VAL	5.5
1	A	303	LEU	5.3
1	B	260	ARG	5.2
1	B	508	LEU	4.9
1	B	300	VAL	4.8
1	A	636	VAL	4.7
1	B	506	PRO	4.7
1	A	900	MET	4.6
1	B	899	ASP	4.5
1	B	303	LEU	4.5
1	B	819	ILE	4.5
1	A	301	GLY	4.2
1	A	251	LYS	4.2
1	B	514	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	903	PHE	4.1
1	A	300	VAL	3.9
1	B	507	ASN	3.8
1	B	503	LEU	3.8
1	B	251	LYS	3.8
1	B	502	ALA	3.7
1	A	897	LEU	3.6
3	F	101	DG	3.6
1	B	610	GLY	3.5
1	A	46	ALA	3.5
1	A	504	HIS	3.5
1	A	262	ILE	3.4
1	B	857	LEU	3.4
1	B	509	SER	3.4
1	B	504	HIS	3.4
1	A	506	PRO	3.4
1	B	46	ALA	3.4
1	B	499	ILE	3.4
1	B	543	PHE	3.3
1	A	641	PHE	3.3
1	A	901	PHE	3.2
1	B	301	GLY	3.2
1	A	503	LEU	3.1
1	B	530	ILE	3.1
1	B	898	PHE	3.1
1	B	513	PRO	3.1
1	B	902	ASP	3.1
1	A	302	LYS	3.1
3	D	101	DG	3.1
1	B	515	ASP	3.1
1	A	891	TYR	3.0
1	B	262	ILE	3.0
1	A	612	GLU	3.0
2	E	3	DT	3.0
1	A	902	ASP	3.0
3	F	102	DC	2.9
1	A	819	ILE	2.9
1	B	498	ILE	2.9
1	B	1	MET	2.8
1	B	511	ASP	2.8
1	A	898	PHE	2.8
1	B	641	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	900	MET	2.8
1	A	611	THR	2.8
1	B	640	LYS	2.8
1	A	642	ARG	2.7
1	A	818	ASN	2.7
1	B	897	LEU	2.7
1	A	646	HIS	2.7
1	B	516	VAL	2.7
1	B	523	SER	2.7
3	D	102	DC	2.7
1	A	502	ALA	2.7
1	B	520	PHE	2.7
1	A	893	LYS	2.7
1	B	261	GLU	2.6
1	A	25	ARG	2.6
1	B	642	ARG	2.6
1	A	45	GLN	2.6
1	B	390	PRO	2.6
1	B	636	VAL	2.6
1	B	612	GLU	2.5
1	B	637	GLY	2.5
1	A	508	LEU	2.5
1	A	837	GLU	2.5
1	B	646	HIS	2.5
1	B	820	ASP	2.4
1	B	535	ALA	2.4
1	B	250	VAL	2.4
1	B	518	TYR	2.4
1	B	531	LYS	2.4
1	B	505	ASN	2.4
1	B	192	ASP	2.4
1	B	538	LEU	2.4
1	A	505	ASN	2.4
1	B	501	GLU	2.3
1	A	857	LEU	2.3
1	A	514	LEU	2.3
1	B	533	LEU	2.3
1	B	527	LYS	2.3
1	B	522	PHE	2.2
1	A	510	VAL	2.2
1	B	517	ASP	2.2
1	B	170	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	467	ARG	2.2
1	B	299	ASN	2.2
1	B	302	LYS	2.2
1	B	818	ASN	2.2
1	A	895	ALA	2.2
1	A	639	SER	2.2
1	B	467	ARG	2.2
1	A	250	VAL	2.2
1	B	550	VAL	2.2
1	B	45	GLN	2.2
1	B	611	THR	2.2
1	B	512	GLU	2.1
1	B	525	GLU	2.1
1	B	526	ILE	2.1
1	B	638	GLU	2.1
1	A	1	MET	2.1
1	A	899	ASP	2.1
1	B	684	ASP	2.1
1	B	384	ARG	2.1
1	B	529	LYS	2.1
1	B	542	LEU	2.1
1	A	199	MET	2.0
1	A	47	THR	2.0
1	A	610	GLY	2.0
1	B	633	ILE	2.0
1	A	892	GLU	2.0
1	B	645	ASN	2.0
1	B	532	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	G35	E	4	22/23	0.86	0.19	39,51,59,61	0
2	G35	C	4	22/23	0.92	0.13	35,46,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	908	5/5	0.84	0.16	78,79,80,80	0
4	SO4	B	907	5/5	0.90	0.14	70,70,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.