Full wwPDB X-ray Structure Validation Report (i)

Jul 25, 2023 – 12:01 AM EDT

PDB ID	:	1ZQM
Title	:	DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF MNCL2 (15 MILLIMOLAR)
Authors	:	Pelletier, H.; Sawaya, M.R.
Deposited on	:	1996-04-12
Resolution	:	3.20 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:

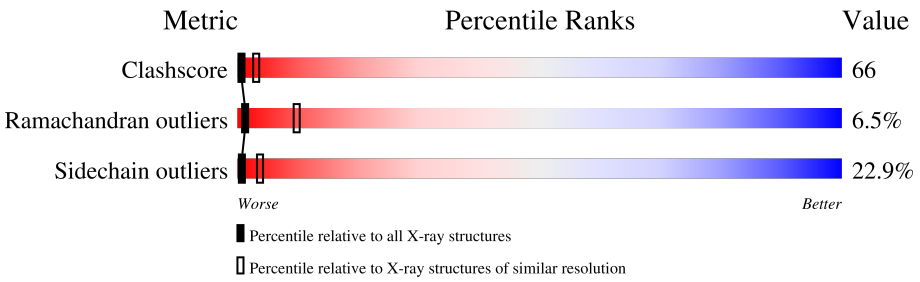
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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%

Mol	Chain	Length	Quality of chain
1	T	8	25% 75%
2	P	7	14% 86%
3	A	335	20% 47% 25% 5% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3058 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	8	145	69	27	42	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	7	144	69	24	44	7	0	0	0

- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	327	2623	1657	458	499	9	18	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	3	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	T	15	15	15	0	0
5	P	21	21	21	0	0
5	A	107	107	107	0	0

3 Residue-property plots (i)

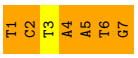
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain T:

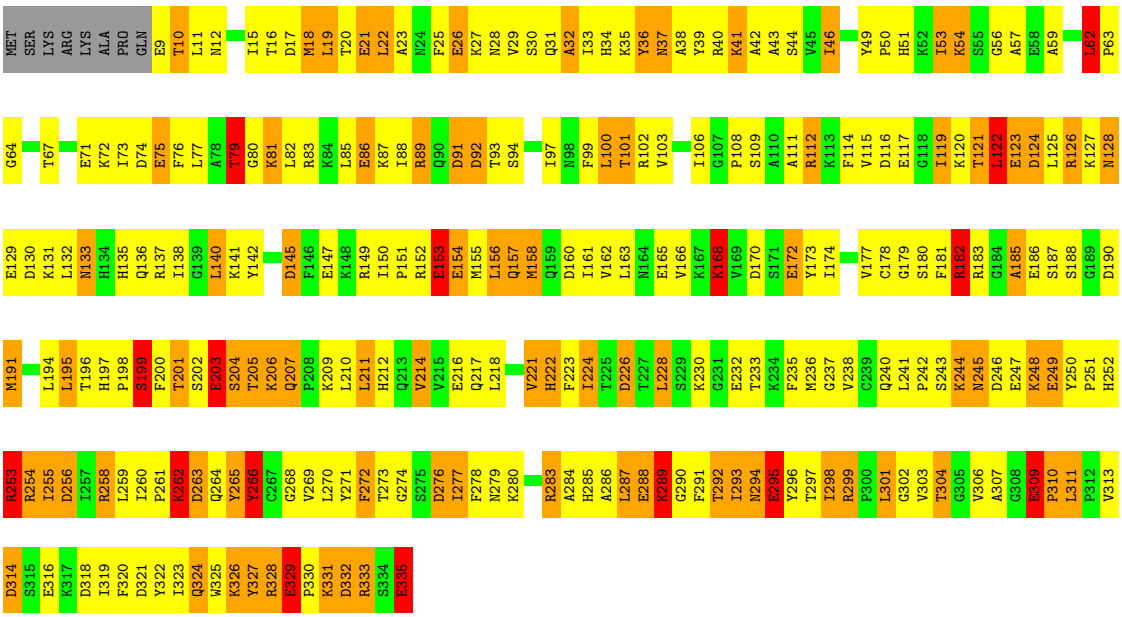
• Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3')

Chain P:



• Molecule 3: PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7))

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	178.88Å 57.63Å 48.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 9.79 – 2.64	Depositor EDS
% Data completeness (in resolution range)	70.0 (20.00-3.20) 65.7 (9.79-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.63Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.149 , (Not available) 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 202.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	T	2.23	7/162 (4.3%)	2.79	8/249 (3.2%)
2	P	2.43	8/160 (5.0%)	3.32	10/243 (4.1%)
3	A	1.17	24/2672 (0.9%)	1.81	66/3590 (1.8%)
All	All	1.35	39/2994 (1.3%)	2.00	84/4082 (2.1%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DA	C3'-O3'	-12.36	1.27	1.44
1	T	6	DG	C3'-O3'	-10.06	1.30	1.44
2	P	2	DC	C1'-N1	8.78	1.60	1.49
1	T	1	DC	C3'-O3'	8.62	1.55	1.44
3	A	147	GLU	CD-OE2	7.58	1.33	1.25
3	A	153	GLU	CD-OE2	7.47	1.33	1.25
1	T	5	DA	P-O5'	6.93	1.66	1.59
3	A	249	GLU	CD-OE2	6.69	1.33	1.25
3	A	86	GLU	CD-OE1	6.62	1.32	1.25
3	A	309	GLU	CD-OE2	6.46	1.32	1.25
3	A	295	GLU	CD-OE2	6.39	1.32	1.25
1	T	4	DT	C5'-C4'	6.32	1.58	1.51
3	A	75	GLU	CD-OE1	6.23	1.32	1.25
3	A	216	GLU	CD-OE2	6.14	1.32	1.25
3	A	335	GLU	CD-OE2	6.06	1.32	1.25
3	A	71	GLU	CD-OE1	6.04	1.32	1.25
3	A	329	GLU	CD-OE2	6.04	1.32	1.25
3	A	154	GLU	CD-OE2	6.00	1.32	1.25
3	A	172	GLU	CD-OE2	5.80	1.32	1.25
3	A	203	GLU	CD-OE1	5.79	1.32	1.25
1	T	2	DA	C3'-O3'	5.76	1.51	1.44
3	A	288	GLU	CD-OE2	5.75	1.31	1.25
1	T	4	DT	P-O5'	5.72	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	123	GLU	CD-OE1	5.66	1.31	1.25
3	A	129	GLU	CD-OE1	5.66	1.31	1.25
2	P	5	DA	C3'-C2'	5.60	1.58	1.52
3	A	26	GLU	CD-OE1	5.54	1.31	1.25
3	A	117	GLU	CD-OE2	5.41	1.31	1.25
3	A	186	GLU	CD-OE1	5.31	1.31	1.25
3	A	9	GLU	CD-OE2	5.27	1.31	1.25
2	P	3	DT	C5-C6	5.26	1.38	1.34
3	A	247	GLU	CD-OE1	5.25	1.31	1.25
2	P	6	DT	C4-O4	-5.18	1.18	1.23
3	A	21	GLU	CD-OE1	5.16	1.31	1.25
3	A	232	GLU	CD-OE2	5.11	1.31	1.25
2	P	5	DA	O3'-P	-5.09	1.55	1.61
2	P	4	DA	C3'-O3'	-5.08	1.37	1.44
2	P	2	DC	C3'-O3'	-5.04	1.37	1.44
1	T	5	DA	C5'-C4'	5.02	1.56	1.51

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	1	DT	C6-N1-C1'	-22.34	86.89	120.40
2	P	1	DT	C2-N1-C1'	20.62	151.19	118.20
2	P	7	DG	C8-N9-C1'	20.50	153.65	127.00
2	P	7	DG	C4-N9-C1'	-20.19	100.25	126.50
1	T	6	DG	C8-N9-C1'	19.33	152.12	127.00
1	T	6	DG	C4-N9-C1'	-18.68	102.22	126.50
1	T	7	DA	C8-N9-C1'	15.66	155.89	127.70
1	T	7	DA	C4-N9-C1'	-15.64	98.14	126.30
2	P	5	DA	C4-N9-C1'	13.20	150.07	126.30
2	P	5	DA	C8-N9-C1'	-13.09	104.13	127.70
1	T	4	DT	C6-N1-C1'	-13.03	100.85	120.40
3	A	253	ARG	NE-CZ-NH1	12.66	126.63	120.30
2	P	2	DC	C2-N1-C1'	11.79	131.76	118.80
1	T	4	DT	C2-N1-C1'	11.71	136.93	118.20
3	A	190	ASP	CB-CG-OD2	-11.10	108.31	118.30
2	P	2	DC	C6-N1-C1'	-10.50	108.20	120.80
3	A	190	ASP	CB-CG-OD1	10.34	127.60	118.30
3	A	182	ARG	NE-CZ-NH1	9.82	125.21	120.30
3	A	258	ARG	NE-CZ-NH1	9.59	125.09	120.30
2	P	6	DT	C6-N1-C1'	-8.77	107.25	120.40
3	A	112	ARG	NE-CZ-NH2	-8.49	116.06	120.30
3	A	256	ASP	CB-CG-OD2	-8.42	110.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	6	DT	C2-N1-C1'	8.09	131.15	118.20
3	A	333	ARG	NE-CZ-NH1	7.91	124.25	120.30
3	A	112	ARG	NE-CZ-NH1	7.89	124.25	120.30
3	A	332	ASP	CB-CG-OD1	-7.83	111.26	118.30
3	A	314	ASP	CB-CG-OD1	-7.76	111.31	118.30
1	T	5	DA	C4-N9-C1'	-7.72	112.39	126.30
1	T	5	DA	C8-N9-C1'	7.39	141.00	127.70
3	A	299	ARG	NE-CZ-NH1	7.25	123.92	120.30
3	A	253	ARG	CD-NE-CZ	7.23	133.72	123.60
3	A	246	ASP	CB-CG-OD1	-7.17	111.85	118.30
3	A	256	ASP	CB-CG-OD1	7.10	124.69	118.30
3	A	266	TYR	CA-CB-CG	-7.06	99.98	113.40
3	A	116	ASP	CB-CG-OD2	-7.02	111.98	118.30
3	A	124	ASP	CB-CG-OD2	-6.98	112.02	118.30
3	A	130	ASP	CB-CG-OD1	6.93	124.54	118.30
3	A	74	ASP	CB-CG-OD1	6.89	124.50	118.30
3	A	222	HIS	CA-CB-CG	-6.88	101.90	113.60
3	A	226	ASP	CB-CG-OD1	6.86	124.47	118.30
3	A	224	ILE	CA-CB-CG1	-6.74	98.19	111.00
3	A	130	ASP	CB-CG-OD2	-6.62	112.34	118.30
3	A	318	ASP	CB-CG-OD2	-6.61	112.35	118.30
3	A	79	THR	CA-CB-CG2	-6.49	103.32	112.40
3	A	263	ASP	CB-CG-OD2	-6.44	112.51	118.30
3	A	40	ARG	NE-CZ-NH1	6.42	123.51	120.30
3	A	258	ARG	NE-CZ-NH2	-6.30	117.15	120.30
3	A	314	ASP	CB-CG-OD2	6.28	123.95	118.30
3	A	226	ASP	CB-CG-OD2	-6.12	112.79	118.30
3	A	195	LEU	CA-CB-CG	-6.11	101.25	115.30
3	A	17	ASP	CB-CG-OD2	6.05	123.74	118.30
3	A	57	ALA	CB-CA-C	-6.04	101.05	110.10
3	A	182	ARG	NE-CZ-NH2	-6.03	117.29	120.30
3	A	253	ARG	NE-CZ-NH2	-5.96	117.32	120.30
3	A	122	LEU	CB-CG-CD2	-5.94	100.90	111.00
3	A	57	ALA	N-CA-CB	-5.93	101.79	110.10
3	A	332	ASP	CB-CG-OD2	5.90	123.61	118.30
3	A	17	ASP	CB-CG-OD1	-5.86	113.03	118.30
3	A	160	ASP	CB-CG-OD2	-5.85	113.03	118.30
3	A	283	ARG	NE-CZ-NH1	5.80	123.20	120.30
3	A	321	ASP	CB-CG-OD2	-5.79	113.08	118.30
3	A	74	ASP	CB-CG-OD2	-5.76	113.12	118.30
3	A	254	ARG	NE-CZ-NH1	5.69	123.14	120.30
3	A	91	ASP	CB-CG-OD2	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	170	ASP	CB-CG-OD2	-5.54	113.31	118.30
3	A	40	ARG	N-CA-CB	5.54	120.57	110.60
3	A	246	ASP	CB-CG-OD2	5.43	123.19	118.30
3	A	116	ASP	CB-CG-OD1	5.39	123.15	118.30
3	A	276	ASP	CB-CG-OD2	-5.38	113.46	118.30
3	A	168	LYS	N-CA-CB	5.36	120.25	110.60
3	A	156	LEU	CA-CB-CG	-5.28	103.17	115.30
3	A	157	GLN	CB-CA-C	5.28	120.95	110.40
3	A	254	ARG	NE-CZ-NH2	-5.25	117.67	120.30
3	A	158	MET	CG-SD-CE	-5.25	91.81	100.20
3	A	157	GLN	N-CA-CB	5.23	120.02	110.60
3	A	53	ILE	CB-CA-C	5.20	122.00	111.60
3	A	62	LEU	C-N-CD	-5.12	109.33	120.60
3	A	170	ASP	CB-CG-OD1	5.12	122.91	118.30
3	A	89	ARG	NE-CZ-NH1	5.11	122.85	120.30
3	A	145	ASP	CB-CG-OD2	-5.07	113.73	118.30
3	A	72	LYS	CB-CA-C	5.02	120.44	110.40
3	A	222	HIS	N-CA-CB	5.01	119.62	110.60
3	A	126	ARG	NE-CZ-NH2	-5.01	117.80	120.30
3	A	93	THR	CA-CB-CG2	-5.01	105.39	112.40

There are no chirality outliers.

There are no planarity outliers.

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	T	145	0	80	6	0
2	P	144	0	81	18	0
3	A	2623	0	2641	349	0
4	A	3	0	0	0	0
5	A	107	0	0	17	0
5	P	21	0	0	2	0
5	T	15	0	0	2	0
All	All	3058	0	2802	370	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 66.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.48	1.11
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.35	1.09
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.30	1.08
2:P:6:DT:H2"	2:P:7:DG:H5"	1.10	1.06
3:A:245:ASN:HD22	3:A:245:ASN:N	1.54	1.04
3:A:245:ASN:H	3:A:245:ASN:ND2	1.57	1.02
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.45	0.99
3:A:31:GLN:HE21	3:A:112:ARG:HH12	0.98	0.96
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.45	0.96
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.47	0.96
2:P:5:DA:H2"	2:P:6:DT:H5"	1.49	0.95
3:A:243:SER:HB3	3:A:249:GLU:HA	1.48	0.95
1:T:6:DG:H2"	1:T:7:DA:C8	2.04	0.92
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.12	0.90
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.54	0.90
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.03	0.89
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.36	0.88
3:A:152:ARG:HA	3:A:155:MET:HB2	1.56	0.87
2:P:6:DT:C2'	2:P:7:DG:H5"	2.02	0.87
2:P:5:DA:H2"	2:P:6:DT:C5'	2.05	0.86
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.57	0.86
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.10	0.85
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.08	0.84
3:A:218:LEU:HD23	3:A:224:ILE:HD11	1.59	0.83
3:A:201:THR:HA	3:A:261:PRO:HB3	1.60	0.83
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.44	0.83
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.60	0.82
3:A:201:THR:HA	3:A:261:PRO:CB	2.08	0.82
3:A:128:ASN:N	3:A:128:ASN:HD22	1.75	0.82
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.63	0.81
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.15	0.80
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.17	0.80
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.64	0.80
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.17	0.79
3:A:330:PRO:HA	3:A:333:ARG:CG	2.12	0.79
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.12	0.79
3:A:18:MET:O	3:A:21:GLU:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.77	0.78
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.66	0.78
3:A:217:GLN:HE21	3:A:217:GLN:HA	1.46	0.77
3:A:243:SER:CB	3:A:249:GLU:HA	2.16	0.75
3:A:165:GLU:CB	3:A:217:GLN:HG3	2.15	0.75
3:A:138:ILE:HD12	3:A:228:LEU:CD1	2.17	0.74
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.21	0.74
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.68	0.74
3:A:92:ASP:HB3	5:A:629:HOH:O	1.87	0.74
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.69	0.73
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.03	0.73
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.70	0.72
3:A:162:VAL:O	3:A:166:VAL:HG23	1.90	0.72
2:P:4:DA:H5'	5:P:563:HOH:O	1.89	0.71
3:A:26:GLU:HA	3:A:30:SER:OG	1.89	0.71
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.22	0.70
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.06	0.70
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.88	0.70
3:A:270:LEU:HD22	3:A:319:ILE:HD13	1.73	0.70
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.72	0.70
3:A:289:LYS:HD3	3:A:289:LYS:N	2.05	0.70
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.72	0.69
3:A:138:ILE:HD12	3:A:228:LEU:HD12	1.74	0.69
3:A:294:ASN:O	3:A:296:TYR:N	2.26	0.69
3:A:165:GLU:HA	3:A:168:LYS:CG	2.22	0.69
3:A:59:ALA:O	3:A:62:LEU:HB2	1.91	0.69
3:A:76:PHE:HD1	3:A:77:LEU:HD12	1.58	0.69
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.75	0.68
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.08	0.68
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.74	0.68
3:A:103:VAL:HB	3:A:106:ILE:CD1	2.18	0.67
3:A:128:ASN:N	3:A:128:ASN:ND2	2.39	0.67
3:A:331:LYS:HG2	3:A:332:ASP:N	2.05	0.67
3:A:82:LEU:HD23	3:A:85:LEU:CB	2.22	0.67
3:A:22:LEU:HD22	3:A:85:LEU:HD13	1.77	0.67
3:A:154:GLU:O	3:A:158:MET:HE2	1.95	0.67
3:A:214:VAL:O	3:A:218:LEU:HD13	1.95	0.67
3:A:35:LYS:O	3:A:38:ALA:HB3	1.95	0.66
3:A:285:HIS:NE2	5:A:574:HOH:O	2.28	0.66
3:A:140:LEU:HD12	3:A:140:LEU:O	1.96	0.66
3:A:295:GLU:N	3:A:295:GLU:OE1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.24	0.66
3:A:306:VAL:HG22	5:A:632:HOH:O	1.95	0.66
3:A:26:GLU:HB3	3:A:32:ALA:HB3	1.77	0.66
3:A:83:ARG:O	3:A:86:GLU:N	2.29	0.66
3:A:211:LEU:HB3	3:A:212:HIS:HD2	1.61	0.66
1:T:1:DC:H2"	1:T:2:DA:OP2	1.93	0.65
3:A:18:MET:CE	3:A:76:PHE:HB2	2.26	0.65
3:A:121:THR:HG23	3:A:124:ASP:CG	2.15	0.65
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.65
3:A:128:ASN:HB3	3:A:131:LYS:HG3	1.79	0.65
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.11	0.65
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.32	0.65
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.27	0.64
3:A:243:SER:OG	3:A:249:GLU:HG3	1.98	0.64
3:A:12:ASN:HD21	3:A:53:ILE:H	1.44	0.64
3:A:79:THR:O	3:A:81:LYS:N	2.30	0.64
3:A:15:ILE:CG2	3:A:46:ILE:HD11	2.28	0.63
3:A:56:GLY:O	3:A:59:ALA:N	2.32	0.63
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.81	0.63
3:A:141:LYS:HE2	3:A:142:TYR:OH	1.98	0.63
3:A:41:LYS:HD3	3:A:42:ALA:H	1.64	0.62
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.81	0.62
3:A:99:PHE:O	3:A:102:ARG:HG3	1.99	0.62
3:A:245:ASN:HD22	3:A:245:ASN:H	0.74	0.62
3:A:12:ASN:HA	5:A:549:HOH:O	2.00	0.62
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.34	0.62
3:A:111:ALA:O	3:A:115:VAL:HG23	1.99	0.62
3:A:150:ILE:N	3:A:188:SER:O	2.31	0.62
3:A:82:LEU:CD2	3:A:85:LEU:HB2	2.26	0.62
3:A:200:PHE:O	3:A:262:LYS:N	2.32	0.62
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.34	0.61
3:A:248:LYS:O	3:A:248:LYS:HG2	2.00	0.61
3:A:253:ARG:NH1	5:A:503:HOH:O	2.34	0.60
3:A:211:LEU:HB3	3:A:212:HIS:CD2	2.37	0.60
3:A:133:ASN:O	3:A:137:ARG:HG3	2.01	0.60
3:A:266:TYR:HA	3:A:269:VAL:HB	1.84	0.60
3:A:127:LYS:HE3	3:A:127:LYS:HA	1.83	0.60
2:P:6:DT:H5'	5:P:561:HOH:O	2.02	0.60
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.82	0.60
3:A:205:THR:HA	5:A:609:HOH:O	2.02	0.60
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:295:GLU:HA	5:A:580:HOH:O	2.01	0.59
3:A:316:GLU:O	3:A:320:PHE:HD1	1.85	0.59
3:A:22:LEU:HD22	3:A:85:LEU:CD1	2.31	0.59
3:A:120:LYS:N	3:A:124:ASP:OD2	2.29	0.59
3:A:211:LEU:HD12	3:A:211:LEU:O	2.02	0.59
3:A:201:THR:CA	3:A:261:PRO:HB3	2.32	0.59
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.83	0.59
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.85	0.58
3:A:323:ILE:O	3:A:324:GLN:HG2	2.03	0.58
3:A:152:ARG:CA	3:A:155:MET:HB2	2.31	0.58
3:A:286:ALA:O	3:A:291:PHE:N	2.35	0.58
1:T:4:DT:H71	5:T:645:HOH:O	2.02	0.58
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.39	0.58
3:A:181:PHE:HD1	5:A:530:HOH:O	1.86	0.58
3:A:254:ARG:CZ	3:A:254:ARG:HB3	2.34	0.58
3:A:75:GLU:O	3:A:79:THR:HG23	2.04	0.58
3:A:82:LEU:HD22	3:A:85:LEU:HD22	1.86	0.57
3:A:142:TYR:CE2	3:A:238:VAL:HG11	2.38	0.57
3:A:309:GLU:N	3:A:309:GLU:OE1	2.37	0.57
2:P:5:DA:C2'	2:P:6:DT:H5"	2.27	0.57
3:A:73:ILE:O	3:A:77:LEU:HD13	2.04	0.57
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.05	0.57
3:A:34:HIS:O	3:A:38:ALA:N	2.34	0.57
3:A:201:THR:HA	3:A:261:PRO:CA	2.34	0.57
3:A:31:GLN:N	5:A:623:HOH:O	2.29	0.57
3:A:255:ILE:HG12	3:A:256:ASP:N	2.19	0.57
3:A:180:SER:CA	3:A:183:ARG:HH21	2.17	0.57
3:A:149:ARG:NH2	3:A:188:SER:HA	2.19	0.57
3:A:15:ILE:CB	3:A:46:ILE:HD11	2.35	0.56
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.87	0.56
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.41	0.56
3:A:33:ILE:O	3:A:36:TYR:HD2	1.89	0.56
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.15	0.56
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.87	0.55
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.21	0.55
3:A:196:THR:OG1	3:A:197:HIS:N	2.40	0.55
3:A:53:ILE:O	3:A:54:LYS:HD2	2.06	0.55
3:A:15:ILE:HG22	3:A:19:LEU:HD22	1.88	0.55
3:A:38:ALA:O	3:A:41:LYS:HD3	2.07	0.55
3:A:123:GLU:O	3:A:127:LYS:HG2	2.07	0.55
3:A:108:PRO:O	3:A:112:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:152:ARG:NH2	3:A:181:PHE:O	2.34	0.54
3:A:278:PHE:HB2	3:A:333:ARG:O	2.07	0.54
1:T:6:DG:O6	2:P:2:DC:N3	2.41	0.54
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.37	0.54
3:A:83:ARG:O	3:A:87:LYS:N	2.35	0.54
3:A:122:LEU:HD22	3:A:126:ARG:NH1	2.22	0.54
3:A:245:ASN:N	3:A:245:ASN:ND2	2.30	0.54
3:A:271:TYR:HB2	5:A:580:HOH:O	2.07	0.54
3:A:240:GLN:NE2	3:A:252:HIS:CE1	2.75	0.54
3:A:328:ARG:O	3:A:333:ARG:NE	2.26	0.54
3:A:264:GLN:NE2	3:A:297:THR:HG23	2.23	0.53
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.73	0.53
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.89	0.53
3:A:327:TYR:HD1	3:A:328:ARG:N	2.07	0.53
3:A:180:SER:HA	3:A:183:ARG:HH21	1.73	0.53
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.39	0.53
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.90	0.53
3:A:211:LEU:HD12	3:A:211:LEU:C	2.29	0.53
3:A:276:ASP:O	3:A:280:LYS:HG3	2.09	0.53
3:A:328:ARG:HB2	3:A:333:ARG:CD	2.39	0.53
2:P:6:DT:H2'	2:P:7:DG:C8	2.44	0.53
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.44	0.53
3:A:124:ASP:O	3:A:128:ASN:ND2	2.41	0.53
3:A:101:THR:HA	3:A:106:ILE:HG22	1.91	0.52
3:A:103:VAL:O	3:A:106:ILE:HB	2.09	0.52
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.55	0.52
3:A:82:LEU:CD2	3:A:85:LEU:HD22	2.39	0.52
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.90	0.52
3:A:240:GLN:NE2	3:A:250:TYR:O	2.41	0.52
2:P:5:DA:H2"	2:P:6:DT:H5'	1.89	0.52
3:A:15:ILE:O	3:A:19:LEU:HB2	2.09	0.52
3:A:266:TYR:O	3:A:270:LEU:HB2	2.09	0.52
3:A:11:LEU:HD23	3:A:11:LEU:H	1.75	0.52
3:A:183:ARG:NH2	5:A:615:HOH:O	2.43	0.52
3:A:274:GLY:O	3:A:278:PHE:HD2	1.93	0.52
3:A:288:GLU:O	3:A:290:GLY:N	2.43	0.52
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.54	0.52
3:A:212:HIS:CD2	3:A:212:HIS:N	2.75	0.52
3:A:259:LEU:O	3:A:260:ILE:HD13	2.10	0.52
3:A:288:GLU:C	3:A:290:GLY:H	2.14	0.52
3:A:195:LEU:O	3:A:260:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:218:LEU:HD23	3:A:224:ILE:CD1	2.37	0.51
3:A:81:LYS:NZ	3:A:86:GLU:HB2	2.26	0.51
3:A:158:MET:O	3:A:162:VAL:HG23	2.11	0.51
3:A:108:PRO:O	3:A:111:ALA:HB3	2.10	0.51
3:A:121:THR:HG23	3:A:124:ASP:OD1	2.11	0.51
3:A:217:GLN:O	3:A:221:VAL:HG13	2.11	0.51
3:A:284:ALA:O	3:A:287:LEU:HB2	2.11	0.51
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.41	0.51
3:A:254:ARG:HB3	3:A:254:ARG:NH1	2.26	0.51
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.41	0.50
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.45	0.50
3:A:12:ASN:OD1	3:A:51:HIS:O	2.29	0.50
3:A:265:TYR:CE2	3:A:269:VAL:HG21	2.47	0.50
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.79	0.50
3:A:100:LEU:O	3:A:106:ILE:HG21	2.12	0.50
3:A:270:LEU:HD22	3:A:319:ILE:CD1	2.40	0.50
3:A:240:GLN:HA	5:A:568:HOH:O	2.11	0.50
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.42	0.50
2:P:6:DT:H5'	2:P:6:DT:H6	1.77	0.50
3:A:179:GLY:O	3:A:182:ARG:HB3	2.11	0.50
3:A:41:LYS:HD3	3:A:42:ALA:N	2.27	0.50
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.46	0.50
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.40	0.50
3:A:127:LYS:HD2	3:A:127:LYS:N	2.27	0.49
3:A:133:ASN:O	3:A:137:ARG:N	2.45	0.49
3:A:254:ARG:NH1	3:A:255:ILE:N	2.60	0.49
3:A:79:THR:C	3:A:81:LYS:H	2.16	0.49
3:A:218:LEU:HB3	3:A:224:ILE:HG13	1.95	0.49
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.76	0.49
3:A:30:SER:HB3	5:A:555:HOH:O	2.13	0.49
3:A:204:SER:O	3:A:206:LYS:N	2.46	0.49
3:A:207:GLN:O	3:A:210:LEU:HB2	2.13	0.49
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.41	0.49
3:A:163:LEU:N	3:A:163:LEU:HD23	2.23	0.49
3:A:302:GLY:N	3:A:307:ALA:HB2	2.26	0.49
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.95	0.48
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.60	0.48
3:A:27:LYS:HG3	3:A:28:ASN:ND2	2.28	0.48
3:A:121:THR:O	3:A:124:ASP:HB2	2.12	0.48
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.79	0.48
3:A:203:GLU:O	3:A:205:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:319:ILE:O	3:A:322:TYR:HB2	2.13	0.48
2:P:6:DT:C2'	2:P:7:DG:C8	2.97	0.48
3:A:19:LEU:O	3:A:22:LEU:HB2	2.14	0.48
3:A:25:PHE:CD2	3:A:88:ILE:HD11	2.49	0.48
3:A:73:ILE:CG2	3:A:77:LEU:HD22	2.42	0.48
3:A:77:LEU:N	3:A:77:LEU:CD1	2.77	0.48
3:A:56:GLY:O	3:A:59:ALA:HB3	2.13	0.47
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.48	0.47
2:P:1:DT:C2'	2:P:2:DC:C6	2.97	0.47
3:A:180:SER:HB2	3:A:185:ALA:CB	2.45	0.47
3:A:212:HIS:CD2	3:A:212:HIS:H	2.31	0.47
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.96	0.47
3:A:41:LYS:CE	3:A:64:GLY:HA3	2.38	0.47
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.42	0.47
3:A:29:VAL:HG21	3:A:94:SER:CB	2.45	0.47
3:A:149:ARG:HH21	3:A:187:SER:C	2.18	0.47
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.80	0.47
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.78	0.46
3:A:237:GLY:O	3:A:254:ARG:NH1	2.48	0.46
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.41	0.46
3:A:323:ILE:C	3:A:324:GLN:HG2	2.33	0.46
3:A:158:MET:HG2	3:A:223:PHE:CZ	2.51	0.46
3:A:173:TYR:O	3:A:174:ILE:HG12	2.15	0.46
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.97	0.46
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.42	0.46
3:A:133:ASN:H	3:A:136:GLN:HE21	1.64	0.46
3:A:158:MET:HG3	3:A:241:LEU:HD21	1.97	0.46
3:A:254:ARG:CA	3:A:254:ARG:HH11	2.28	0.46
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.95	0.46
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.98	0.46
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.25	0.46
3:A:99:PHE:HD2	3:A:100:LEU:HD13	1.81	0.46
3:A:265:TYR:HD2	3:A:266:TYR:CE1	2.33	0.46
3:A:326:LYS:HG3	3:A:326:LYS:O	2.15	0.46
3:A:18:MET:HE1	3:A:76:PHE:CB	2.44	0.45
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.26	0.45
3:A:133:ASN:ND2	3:A:135:HIS:H	2.15	0.45
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.97	0.45
3:A:18:MET:HG2	3:A:19:LEU:N	2.27	0.45
3:A:249:GLU:HG3	3:A:250:TYR:H	1.81	0.45
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.79	0.45
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.49	0.45
3:A:200:PHE:CE2	3:A:261:PRO:N	2.85	0.45
3:A:15:ILE:HG21	3:A:46:ILE:CD1	2.46	0.45
3:A:127:LYS:HB2	3:A:128:ASN:HD22	1.82	0.45
3:A:36:TYR:CD2	3:A:37:ASN:N	2.85	0.45
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.29	0.45
3:A:320:PHE:CE2	3:A:328:ARG:HG3	2.51	0.45
1:T:4:DT:H2"	1:T:5:DA:C8	2.52	0.45
5:T:545:HOH:O	3:A:133:ASN:HB2	2.17	0.45
3:A:302:GLY:N	3:A:307:ALA:CB	2.80	0.45
2:P:1:DT:H2"	2:P:2:DC:O4'	2.17	0.45
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.99	0.45
3:A:140:LEU:HD12	3:A:140:LEU:C	2.31	0.45
3:A:156:LEU:HA	3:A:156:LEU:HD23	1.54	0.44
3:A:243:SER:HB3	3:A:249:GLU:CA	2.34	0.44
3:A:249:GLU:CG	3:A:250:TYR:N	2.80	0.44
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.98	0.44
3:A:15:ILE:HG22	3:A:15:ILE:O	2.16	0.44
3:A:258:ARG:NH2	3:A:272:PHE:CZ	2.86	0.44
3:A:79:THR:HG23	3:A:79:THR:H	1.44	0.44
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.41	0.44
3:A:250:TYR:HA	3:A:251:PRO:HD3	1.88	0.44
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.45	0.44
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.96	0.44
3:A:97:ILE:HG23	3:A:111:ALA:HB1	2.00	0.44
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.70	0.44
3:A:149:ARG:NH2	3:A:188:SER:CA	2.80	0.44
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.42	0.43
3:A:112:ARG:O	3:A:115:VAL:HB	2.17	0.43
3:A:154:GLU:C	3:A:158:MET:HE2	2.37	0.43
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.77	0.43
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.43	0.43
3:A:31:GLN:O	3:A:33:ILE:N	2.49	0.43
3:A:102:ARG:HH11	3:A:102:ARG:HD3	1.59	0.43
3:A:152:ARG:O	3:A:155:MET:HB2	2.18	0.43
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.71	0.43
3:A:265:TYR:O	3:A:268:GLY:N	2.51	0.43
3:A:277:ILE:HG13	3:A:335:GLU:HB2	2.00	0.43
3:A:22:LEU:O	3:A:25:PHE:HB3	2.18	0.43
3:A:262:LYS:O	3:A:262:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:243:SER:O	3:A:244:LYS:O	2.37	0.42
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.40	0.42
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.60	0.42
3:A:16:THR:O	3:A:20:THR:HG23	2.19	0.42
3:A:293:ILE:HA	5:A:581:HOH:O	2.18	0.42
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.34	0.42
2:P:1:DT:H2'	2:P:2:DC:C6	2.53	0.42
3:A:54:LYS:HD2	3:A:54:LYS:HA	1.59	0.42
3:A:165:GLU:CA	3:A:168:LYS:HG2	2.33	0.42
3:A:271:TYR:CD2	3:A:272:PHE:N	2.87	0.42
3:A:180:SER:HA	3:A:183:ARG:NH2	2.33	0.42
3:A:286:ALA:HB1	3:A:291:PHE:HB2	2.02	0.42
3:A:266:TYR:HB2	3:A:313:VAL:HG11	2.01	0.42
3:A:331:LYS:CG	3:A:332:ASP:N	2.80	0.42
3:A:25:PHE:CE2	3:A:88:ILE:HD11	2.55	0.41
3:A:29:VAL:HG21	3:A:94:SER:HA	2.01	0.41
3:A:261:PRO:O	3:A:263:ASP:N	2.52	0.41
1:T:7:DA:H61	2:P:1:DT:H3	1.68	0.41
2:P:1:DT:H2"	2:P:2:DC:C6	2.55	0.41
3:A:22:LEU:HD21	3:A:82:LEU:HD21	2.00	0.41
3:A:195:LEU:HG	3:A:196:THR:N	2.35	0.41
3:A:12:ASN:ND2	5:A:624:HOH:O	2.53	0.41
3:A:289:LYS:HD3	3:A:289:LYS:HA	1.50	0.41
3:A:278:PHE:HZ	3:A:320:PHE:HZ	1.69	0.41
3:A:29:VAL:CG2	3:A:94:SER:HA	2.50	0.41
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.20	0.41
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.50	0.41
3:A:62:LEU:HD12	3:A:63:PRO:CD	2.43	0.41
3:A:22:LEU:CD2	3:A:85:LEU:HD13	2.48	0.41
3:A:242:PRO:HB2	5:A:577:HOH:O	2.19	0.41
2:P:5:DA:P	3:A:109:SER:HB3	2.61	0.41
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.74	0.41
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.64	0.41
3:A:205:THR:HG23	3:A:205:THR:O	2.22	0.40
3:A:283:ARG:HG3	5:A:550:HOH:O	2.21	0.40
3:A:302:GLY:H	3:A:307:ALA:HB2	1.86	0.40
3:A:22:LEU:HD21	3:A:82:LEU:CD2	2.52	0.40
3:A:198:PRO:C	3:A:200:PHE:H	2.24	0.40
3:A:301:LEU:HA	3:A:307:ALA:HB3	2.03	0.40
3:A:326:LYS:O	3:A:328:ARG:HG2	2.20	0.40
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:287:LEU:HA	3:A:287:LEU:HD13	1.55	0.40
3:A:303:VAL:O	3:A:303:VAL:HG22	2.22	0.40
3:A:180:SER:HA	3:A:183:ARG:HE	1.86	0.40
3:A:244:LYS:H	3:A:244:LYS:HG2	1.72	0.40
3:A:329:GLU:O	3:A:333:ARG:HG2	2.22	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	A	325/335 (97%)	269 (83%)	35 (11%)	21 (6%)	1 10

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	202	SER
3	A	204	SER
3	A	205	THR
3	A	244	LYS
3	A	265	TYR
3	A	266	TYR
3	A	289	LYS
3	A	295	GLU
3	A	10	THR
3	A	80	GLY
3	A	91	ASP
3	A	262	LYS
3	A	185	ALA
3	A	199	SER
3	A	206	LYS

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Mol	Chain	Res	Type
3	A	222	HIS
3	A	207	GLN
3	A	304	THR
3	A	310	PRO
3	A	309	GLU

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	A	288/295 (98%)	222 (77%)	66 (23%)	1 4

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	36	TYR
3	A	37	ASN
3	A	41	LYS
3	A	44	SER
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	79	THR
3	A	81	LYS
3	A	89	ARG
3	A	92	ASP
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	121	THR
3	A	122	LEU

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Mol	Chain	Res	Type
3	A	128	ASN
3	A	133	ASN
3	A	140	LEU
3	A	145	ASP
3	A	153	GLU
3	A	161	ILE
3	A	168	LYS
3	A	182	ARG
3	A	191	MET
3	A	199	SER
3	A	201	THR
3	A	203	GLU
3	A	211	LEU
3	A	214	VAL
3	A	221	VAL
3	A	226	ASP
3	A	228	LEU
3	A	230	LYS
3	A	233	THR
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	262	LYS
3	A	272	PHE
3	A	277	ILE
3	A	287	LEU
3	A	289	LYS
3	A	292	THR
3	A	293	ILE
3	A	294	ASN
3	A	298	ILE
3	A	301	LEU
3	A	304	THR
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	324	GLN
3	A	325	TRP
3	A	326	LYS
3	A	327	TYR
3	A	328	ARG

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Mol	Chain	Res	Type
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	51	HIS
3	A	128	ASN
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	240	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN

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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.