Full wwPDB X-ray Structure Validation Report (i)

Jul 25, 2023 – 12:23 AM EDT

PDB ID	:	1ZQE
Title	:	DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF CRCL3 (SATURATED SOLUTION)
Authors	:	Pelletier, H.; Sawaya, M.R.
Deposited on	:	1996-04-12
Resolution	:	3.70 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:

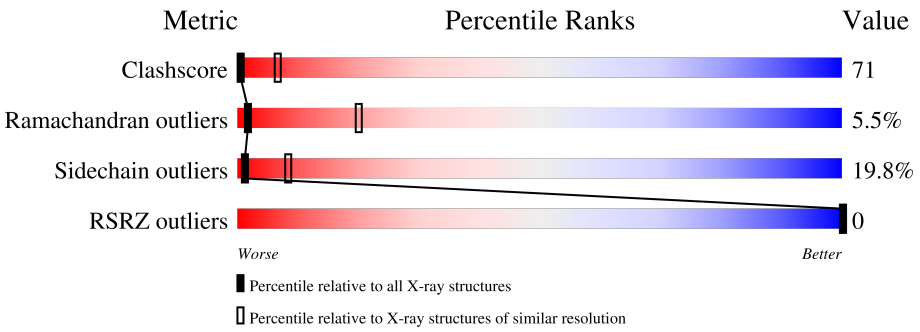
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.70 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	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	T	8	12% 12% 75%
2	P	7	14% 14% 71%
3	A	335	19% 47% 28% . .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3057 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 CHROMIUM ION (three-letter code: CR) (formula: Cr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cr		
4	A	2	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	T	13	13	13	0	0
5	P	22	22	22	0	0
5	A	108	108	108	0	0

3 Residue-property plots (i)

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

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

Chain T: 12% 12% 75%

C1 A2 T3 T4 A5 G6 A7 A8

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

Chain P: 14% 14% 71%

T1 C2 T3 A4 A5 T6 G7

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

Chain A: 19% 47% 28%

MET SER LYS ARG LYS ALA PRO GLN E9 T10 L11 N12 G13 G14 I15 T16 D17 M18 L19 T20 E21 L22 A23 N24 F25 E26 K27 N28 V29 S30 Q31 A32 I33 H34 K35 Y36 N37 A38 Y39 R40 K41 A42 A43 S44 V45 I46 A47 K48 Y49 P50 I53 K54 S55 G56 A57 E58 A59 L62

P63 G64 T67 K68 E71 K72 I73 D74 E75 F76 L77 A78 T79 G80 K81 L82 R83 K84 L85 E86 K87 I88 R89 Q90 D91 D92 T93 S94 I97 L100 T101 R102 V103 I106 G107 P108 S109 A110 A111 R112 K113 F114 V115 D116 E117 G118 I119 K120 T121 L122 E123 D124 L125 R126 K127

N128 E129 D130 K131 L132 N133 H134 H135 Q136 R137 I138 G139 L140 K141 Y142 F143 G144 D145 F146 E147 K148 R149 I150 L151 P152 E153 E154 M155 L156 Q157 M158 Q159 D160 I161 V162 L163 N164 E165 V166 K167 K168 V169 D170 S171 E172 Y173 I174 A175 T176 V177 C178 G179 S180 F181 R182 R183 G184 A185 S188

G189 D190 M191 D192 V193 L194 L195 T196 H197 P198 S199 F200 T201 S202 E203 S204 T205 K206 Q207 P208 K209 L210 L211 H212 Q213 V214 V215 E216 Q217 L218 Q219 K220 V221 H222 F223 I224 T225 D226 T227 L228 S229 K230 G231 E232 F235 M236 G237 V238 C239 Q240 L241 P242 S243 K244 N245 D246 E247 K248 E249

Y250 P251 H252 R253 R254 I255 D256 I257 R258 L259 I260 P261 K262 D263 Q264 Y265 Y266 C267 G268 V269 L270 Y271 F272 T273 G274 S275 D276 I277 F278 N279 K280 N281 M282 R283 A284 H285 A286 L287 E288 K289 G290 F291 T292 I293 N294 E295 Y296 T297 I298 R299 P300 L301 G302 V303 T304 G305 V306 E309 P310

L311 D314 S315 E316 K317 D318 I319 F320 D321 Y322 I323 Q324 W325 K326 Y327 R328 E329 P330 K331 D332 R333 S334 E335

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	178.98Å 57.46Å 47.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 9.97 – 3.78	Depositor EDS
% Data completeness (in resolution range)	74.0 (20.00-3.70) 83.0 (9.97-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.73Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.171 , (Not available) 0.161 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.968	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.13 , 183.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3057	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: CR

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	3.03	17/162 (10.5%)	2.56	8/249 (3.2%)
2	P	2.97	12/160 (7.5%)	3.62	10/243 (4.1%)
3	A	1.22	27/2672 (1.0%)	1.96	74/3590 (2.1%)
All	All	1.52	56/2994 (1.9%)	2.14	92/4082 (2.3%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DA	C3'-O3'	-13.71	1.26	1.44
2	P	5	DA	O3'-P	-11.04	1.48	1.61
1	T	6	DG	C3'-O3'	-9.53	1.31	1.44
1	T	2	DA	C3'-O3'	9.15	1.55	1.44
1	T	3	DT	C4-C5	8.57	1.52	1.45
2	P	5	DA	C3'-C2'	8.20	1.62	1.52
2	P	2	DC	C1'-N1	7.95	1.59	1.49
1	T	1	DC	C3'-O3'	7.60	1.53	1.44
3	A	309	GLU	CD-OE2	7.44	1.33	1.25
1	T	7	DA	N9-C8	-7.20	1.31	1.37
1	T	6	DG	N7-C5	-7.18	1.34	1.39
3	A	147	GLU	CD-OE2	7.15	1.33	1.25
3	A	153	GLU	CD-OE2	7.12	1.33	1.25
3	A	295	GLU	CD-OE2	7.11	1.33	1.25
3	A	75	GLU	CD-OE1	7.08	1.33	1.25
3	A	154	GLU	CD-OE2	6.84	1.33	1.25
3	A	129	GLU	CD-OE1	6.67	1.32	1.25
1	T	4	DT	C3'-O3'	6.67	1.52	1.44
3	A	71	GLU	CD-OE1	6.66	1.32	1.25
3	A	26	GLU	CD-OE1	6.57	1.32	1.25
1	T	7	DA	C1'-N9	-6.56	1.38	1.47
3	A	117	GLU	CD-OE2	6.53	1.32	1.25
3	A	249	GLU	CD-OE2	6.53	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	288	GLU	CD-OE2	6.52	1.32	1.25
1	T	3	DT	C3'-O3'	-6.44	1.35	1.44
3	A	86	GLU	CD-OE1	6.42	1.32	1.25
3	A	172	GLU	CD-OE2	6.32	1.32	1.25
1	T	5	DA	N9-C4	-6.30	1.34	1.37
1	T	5	DA	C1'-N9	-6.29	1.38	1.47
3	A	329	GLU	CD-OE2	6.28	1.32	1.25
3	A	335	GLU	CD-OE2	6.25	1.32	1.25
1	T	4	DT	C4-C5	6.22	1.50	1.45
2	P	4	DA	C6-N1	-6.20	1.31	1.35
3	A	216	GLU	CD-OE2	6.12	1.32	1.25
3	A	192	ASP	CG-OD1	5.99	1.39	1.25
1	T	3	DT	C5'-C4'	-5.87	1.44	1.51
3	A	58	GLU	CD-OE1	5.83	1.32	1.25
3	A	165	GLU	CD-OE2	5.77	1.31	1.25
3	A	123	GLU	CD-OE1	5.76	1.31	1.25
2	P	6	DT	C4-C5	5.70	1.50	1.45
3	A	316	GLU	CD-OE2	5.67	1.31	1.25
2	P	6	DT	N1-C6	5.62	1.42	1.38
2	P	4	DA	C3'-O3'	-5.61	1.36	1.44
1	T	6	DG	O5'-C5'	-5.46	1.28	1.42
3	A	232	GLU	CD-OE2	5.39	1.31	1.25
1	T	2	DA	O3'-P	5.38	1.67	1.61
3	A	247	GLU	CD-OE1	5.31	1.31	1.25
3	A	203	GLU	CD-OE1	5.31	1.31	1.25
3	A	165	GLU	CD-OE1	-5.28	1.19	1.25
2	P	5	DA	N9-C4	5.28	1.41	1.37
3	A	9	GLU	CD-OE2	5.27	1.31	1.25
2	P	5	DA	N3-C4	5.14	1.38	1.34
1	T	7	DA	O4'-C1'	-5.13	1.36	1.42
2	P	6	DT	O4'-C1'	-5.05	1.36	1.42
1	T	3	DT	C5-C7	5.04	1.53	1.50
2	P	5	DA	N9-C8	-5.03	1.33	1.37

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	7	DG	C8-N9-C1'	23.57	157.64	127.00
2	P	7	DG	C4-N9-C1'	-23.37	96.12	126.50
2	P	1	DT	C6-N1-C1'	-19.84	90.64	120.40
2	P	1	DT	C2-N1-C1'	18.39	147.62	118.20
1	T	6	DG	C8-N9-C1'	15.25	146.82	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	6	DG	C4-N9-C1'	-15.15	106.81	126.50
1	T	4	DT	C6-N1-C1'	-15.00	97.90	120.40
1	T	4	DT	C2-N1-C1'	13.89	140.43	118.20
2	P	2	DC	C2-N1-C1'	13.81	134.00	118.80
2	P	6	DT	C6-N1-C1'	-13.73	99.80	120.40
1	T	7	DA	C4-N9-C1'	-13.55	101.91	126.30
2	P	5	DA	C8-N9-C1'	-13.27	103.81	127.70
2	P	5	DA	C4-N9-C1'	12.83	149.40	126.30
2	P	2	DC	C6-N1-C1'	-12.74	105.51	120.80
1	T	7	DA	C8-N9-C1'	12.70	150.57	127.70
2	P	6	DT	C2-N1-C1'	12.27	137.83	118.20
3	A	190	ASP	CB-CG-OD2	-11.89	107.60	118.30
3	A	333	ARG	NE-CZ-NH1	11.45	126.03	120.30
3	A	258	ARG	NE-CZ-NH2	-10.70	114.95	120.30
3	A	190	ASP	CB-CG-OD1	10.20	127.48	118.30
3	A	318	ASP	CB-CG-OD2	-9.19	110.03	118.30
3	A	74	ASP	CB-CG-OD2	-9.15	110.06	118.30
3	A	160	ASP	CB-CG-OD2	-9.11	110.10	118.30
3	A	254	ARG	NE-CZ-NH1	9.07	124.84	120.30
3	A	253	ARG	NE-CZ-NH1	8.61	124.60	120.30
3	A	314	ASP	CB-CG-OD1	-8.41	110.73	118.30
3	A	74	ASP	CB-CG-OD1	8.37	125.83	118.30
3	A	143	PHE	CB-CG-CD2	-8.13	115.11	120.80
3	A	126	ARG	NE-CZ-NH2	-8.07	116.26	120.30
3	A	183	ARG	NE-CZ-NH1	7.99	124.29	120.30
3	A	145	ASP	CB-CG-OD2	-7.85	111.24	118.30
3	A	283	ARG	NE-CZ-NH1	7.85	124.22	120.30
3	A	170	ASP	CB-CG-OD1	7.77	125.29	118.30
3	A	91	ASP	CB-CG-OD1	-7.68	111.39	118.30
3	A	333	ARG	NE-CZ-NH2	-7.67	116.47	120.30
3	A	160	ASP	CB-CG-OD1	7.53	125.07	118.30
3	A	192	ASP	CB-CG-OD1	-7.51	111.54	118.30
3	A	254	ARG	NE-CZ-NH2	-7.27	116.67	120.30
3	A	170	ASP	CB-CG-OD2	-7.20	111.82	118.30
3	A	116	ASP	CB-CG-OD2	-7.13	111.88	118.30
3	A	124	ASP	CB-CG-OD1	7.11	124.70	118.30
3	A	226	ASP	CB-CG-OD1	7.11	124.70	118.30
3	A	227	THR	N-CA-CB	6.97	123.54	110.30
3	A	137	ARG	NE-CZ-NH1	6.89	123.74	120.30
3	A	142	TYR	CB-CG-CD2	-6.85	116.89	121.00
3	A	222	HIS	CA-CB-CG	-6.83	101.99	113.60
3	A	258	ARG	NE-CZ-NH1	6.82	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	40	ARG	NE-CZ-NH1	6.75	123.68	120.30
3	A	283	ARG	NE-CZ-NH2	-6.75	116.93	120.30
3	A	182	ARG	NE-CZ-NH2	-6.74	116.93	120.30
3	A	152	ARG	NE-CZ-NH2	6.72	123.66	120.30
3	A	229	SER	N-CA-CB	6.68	120.53	110.50
3	A	246	ASP	CB-CG-OD1	-6.64	112.32	118.30
3	A	226	ASP	CB-CG-OD2	-6.51	112.44	118.30
3	A	168	LYS	N-CA-CB	6.44	122.19	110.60
3	A	157	GLN	CB-CA-C	6.40	123.19	110.40
3	A	57	ALA	N-CA-CB	-6.34	101.23	110.10
3	A	332	ASP	CB-CG-OD1	-6.31	112.62	118.30
3	A	328	ARG	NE-CZ-NH1	6.30	123.45	120.30
3	A	124	ASP	CB-CG-OD2	-6.24	112.69	118.30
3	A	256	ASP	CB-CG-OD2	-6.21	112.71	118.30
3	A	246	ASP	CB-CG-OD2	6.18	123.87	118.30
3	A	222	HIS	N-CA-CB	6.16	121.69	110.60
3	A	155	MET	CG-SD-CE	6.06	109.90	100.20
3	A	101	THR	CA-CB-CG2	6.05	120.86	112.40
3	A	224	ILE	CA-CB-CG1	-6.00	99.61	111.00
3	A	182	ARG	NE-CZ-NH1	5.94	123.27	120.30
3	A	263	ASP	CB-CG-OD2	-5.94	112.96	118.30
3	A	265	TYR	CB-CG-CD2	5.87	124.52	121.00
3	A	276	ASP	CB-CG-OD2	-5.84	113.04	118.30
3	A	253	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	A	92	ASP	CB-CG-OD1	-5.63	113.23	118.30
3	A	318	ASP	CB-CG-OD1	5.62	123.36	118.30
3	A	151	PRO	N-CA-CB	5.57	109.99	103.30
3	A	102	ARG	CA-CB-CG	-5.53	101.24	113.40
3	A	130	ASP	CB-CG-OD2	-5.53	113.33	118.30
3	A	17	ASP	CB-CA-C	5.51	121.42	110.40
3	A	176	THR	CA-CB-CG2	-5.43	104.80	112.40
3	A	28	ASN	CA-CB-CG	-5.42	101.47	113.40
3	A	62	LEU	CB-CG-CD2	-5.32	101.95	111.00
3	A	116	ASP	CB-CA-C	5.32	121.04	110.40
1	T	2	DA	C4-N9-C1'	-5.26	116.82	126.30
3	A	158	MET	CG-SD-CE	-5.26	91.78	100.20
3	A	266	TYR	CA-CB-CG	-5.25	103.42	113.40
3	A	321	ASP	CB-CG-OD2	-5.22	113.60	118.30
3	A	173	TYR	CD1-CE1-CZ	-5.17	115.14	119.80
3	A	91	ASP	CB-CG-OD2	5.16	122.95	118.30
3	A	264	GLN	N-CA-CB	5.12	119.81	110.60
3	A	64	GLY	C-N-CA	-5.10	108.96	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	2	DA	C8-N9-C1'	5.09	136.87	127.70
3	A	67	THR	CA-CB-CG2	5.06	119.48	112.40
3	A	25	PHE	CB-CG-CD1	-5.04	117.27	120.80

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	5	0
2	P	144	0	81	21	0
3	A	2623	0	2641	380	0
4	A	2	0	0	0	0
5	A	108	0	0	18	0
5	P	22	0	0	4	0
5	T	13	0	0	1	0
All	All	3057	0	2802	403	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 71.

All (403) 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)
2:P:5:DA:H2"	2:P:6:DT:H5"	1.21	1.12
2:P:6:DT:H2"	2:P:7:DG:H5"	1.17	1.09
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.54	1.05
3:A:245:ASN:N	3:A:245:ASN:HD22	1.52	1.00
3:A:243:SER:HB3	3:A:249:GLU:HA	1.41	0.99
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.41	0.99
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.43	0.98
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.28	0.97
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.47	0.97
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:6:DG:H2"	1:T:7:DA:C8	2.01	0.96
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.49	0.94
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.00	0.93
3:A:245:ASN:H	3:A:245:ASN:ND2	1.65	0.92
3:A:259:LEU:HD12	3:A:260:ILE:H	1.35	0.91
3:A:138:ILE:HD12	3:A:228:LEU:CD1	2.01	0.91
2:P:5:DA:H2"	2:P:6:DT:C5'	2.02	0.90
3:A:201:THR:HA	3:A:261:PRO:HB3	1.54	0.89
3:A:197:HIS:ND1	3:A:199:SER:HB3	1.88	0.88
3:A:217:GLN:HE21	3:A:217:GLN:HA	1.41	0.85
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.76	0.84
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.17	0.84
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.59	0.83
3:A:97:ILE:HG23	3:A:111:ALA:HB1	1.61	0.83
3:A:68:LYS:O	3:A:72:LYS:HE2	1.81	0.81
3:A:243:SER:CB	3:A:249:GLU:HA	2.11	0.81
3:A:245:ASN:HD22	3:A:245:ASN:H	0.84	0.81
2:P:6:DT:C2'	2:P:7:DG:H5"	2.08	0.81
3:A:330:PRO:HA	3:A:333:ARG:CG	2.11	0.79
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.17	0.79
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.12	0.79
3:A:165:GLU:HA	3:A:168:LYS:CG	2.11	0.79
2:P:5:DA:C2'	2:P:6:DT:H5"	2.10	0.79
3:A:201:THR:HA	3:A:261:PRO:CB	2.12	0.78
3:A:127:LYS:HB2	3:A:128:ASN:ND2	1.97	0.78
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.66	0.78
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.19	0.78
3:A:209:LYS:HA	3:A:212:HIS:HB2	1.65	0.77
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.20	0.77
3:A:259:LEU:HD12	3:A:260:ILE:N	2.00	0.77
3:A:197:HIS:HD1	3:A:199:SER:HB3	1.47	0.76
3:A:306:VAL:HG22	5:A:632:HOH:O	1.85	0.76
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.00	0.76
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.21	0.75
3:A:152:ARG:HA	3:A:155:MET:HB2	1.68	0.75
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.67	0.75
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.68	0.75
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.69	0.75
3:A:289:LYS:HD3	3:A:289:LYS:N	2.02	0.74
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.70	0.74
3:A:254:ARG:HB3	3:A:254:ARG:NH1	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:250:TYR:HB3	5:A:568:HOH:O	1.88	0.72
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.18	0.72
2:P:5:DA:O5'	3:A:107:GLY:HA3	1.89	0.72
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.25	0.71
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.21	0.71
3:A:92:ASP:HB3	5:A:629:HOH:O	1.90	0.70
2:P:5:DA:H1'	5:P:559:HOH:O	1.89	0.70
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.19	0.70
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.72	0.70
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.21	0.70
3:A:26:GLU:HB3	3:A:32:ALA:HB3	1.73	0.70
3:A:323:ILE:O	3:A:324:GLN:HG2	1.91	0.70
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.74	0.69
3:A:18:MET:CE	3:A:76:PHE:HB2	2.23	0.68
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.74	0.68
3:A:22:LEU:HB3	3:A:39:TYR:CE1	2.28	0.68
3:A:271:TYR:HB2	5:A:580:HOH:O	1.92	0.68
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.23	0.68
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.03	0.68
3:A:150:ILE:HG12	3:A:253:ARG:NH1	2.09	0.68
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.76	0.68
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.23	0.68
3:A:103:VAL:HG11	3:A:106:ILE:HD12	1.76	0.67
3:A:200:PHE:O	3:A:261:PRO:HA	1.95	0.67
3:A:19:LEU:HD23	3:A:43:ALA:HB2	1.77	0.67
3:A:294:ASN:O	3:A:296:TYR:N	2.27	0.67
3:A:103:VAL:CG1	3:A:106:ILE:HD12	2.24	0.67
3:A:162:VAL:O	3:A:166:VAL:HG23	1.94	0.67
3:A:211:LEU:HD12	3:A:211:LEU:O	1.93	0.67
3:A:254:ARG:HB3	3:A:254:ARG:CZ	2.24	0.67
3:A:265:TYR:HD2	3:A:266:TYR:CE1	2.13	0.67
3:A:128:ASN:N	3:A:128:ASN:HD22	1.93	0.67
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.61	0.66
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.30	0.66
3:A:19:LEU:HD23	3:A:43:ALA:CA	2.25	0.66
3:A:41:LYS:HD3	3:A:42:ALA:H	1.60	0.66
2:P:1:DT:H2"	2:P:2:DC:O4'	1.96	0.66
3:A:97:ILE:HG23	3:A:111:ALA:CB	2.24	0.66
3:A:18:MET:HG2	3:A:19:LEU:N	2.07	0.66
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.10	0.66
3:A:299:ARG:CG	3:A:310:PRO:HD3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:25:PHE:CE1	3:A:88:ILE:HG12	2.31	0.65
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.77	0.65
3:A:245:ASN:N	3:A:245:ASN:ND2	2.29	0.65
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.61	0.65
3:A:111:ALA:O	3:A:115:VAL:HG23	1.96	0.65
3:A:286:ALA:O	3:A:291:PHE:N	2.29	0.65
1:T:1:DC:H2"	1:T:2:DA:OP2	1.95	0.65
3:A:319:ILE:O	3:A:322:TYR:HB2	1.97	0.65
3:A:83:ARG:O	3:A:86:GLU:N	2.30	0.65
3:A:18:MET:O	3:A:21:GLU:HB2	1.96	0.64
2:P:7:DG:N3	5:P:643:HOH:O	2.29	0.64
3:A:165:GLU:CA	3:A:168:LYS:HG2	2.25	0.64
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.30	0.64
3:A:180:SER:HA	3:A:183:ARG:HH21	1.63	0.64
3:A:44:SER:O	3:A:47:ALA:HB3	1.97	0.64
3:A:254:ARG:NH2	5:A:639:HOH:O	2.29	0.64
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.80	0.64
3:A:236:MET:HG3	3:A:256:ASP:OD1	1.97	0.64
3:A:327:TYR:HD1	3:A:328:ARG:N	1.95	0.64
3:A:108:PRO:O	3:A:111:ALA:HB3	1.99	0.63
3:A:295:GLU:HA	5:A:580:HOH:O	1.98	0.63
3:A:59:ALA:O	3:A:62:LEU:HB2	1.99	0.63
3:A:174:ILE:O	3:A:195:LEU:HD12	1.98	0.63
3:A:119:ILE:HG21	3:A:125:LEU:HD23	1.80	0.63
3:A:26:GLU:HA	3:A:30:SER:OG	1.98	0.63
3:A:207:GLN:O	3:A:210:LEU:HB2	1.99	0.63
3:A:155:MET:CE	3:A:188:SER:HB2	2.29	0.62
3:A:180:SER:CA	3:A:183:ARG:HH21	2.12	0.62
3:A:299:ARG:HG2	3:A:310:PRO:N	2.13	0.62
3:A:15:ILE:O	3:A:19:LEU:HB2	1.99	0.62
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.80	0.62
2:P:5:DA:H2'	2:P:6:DT:H71	1.82	0.62
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.37	0.62
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.81	0.61
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.31	0.61
3:A:127:LYS:HB2	3:A:128:ASN:HD22	1.64	0.61
3:A:123:GLU:O	3:A:127:LYS:HG2	2.01	0.60
3:A:180:SER:CB	3:A:183:ARG:HH21	2.14	0.60
3:A:239:CYS:SG	3:A:255:ILE:HB	2.42	0.60
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.83	0.60
3:A:270:LEU:HD21	3:A:282:MET:CE	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:THR:CA	3:A:261:PRO:HB3	2.28	0.60
3:A:316:GLU:O	3:A:320:PHE:HD2	1.85	0.60
3:A:22:LEU:HB3	3:A:39:TYR:CD1	2.37	0.60
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.84	0.60
3:A:152:ARG:NH2	3:A:184:GLY:HA2	2.17	0.59
3:A:214:VAL:O	3:A:218:LEU:HD13	2.02	0.59
3:A:248:LYS:O	3:A:248:LYS:HG2	2.01	0.59
3:A:88:ILE:HG22	3:A:89:ARG:N	2.16	0.59
3:A:154:GLU:HB3	5:A:521:HOH:O	2.03	0.59
3:A:183:ARG:HD3	3:A:273:THR:O	2.03	0.59
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.85	0.59
3:A:263:ASP:O	3:A:264:GLN:HG2	2.03	0.59
3:A:326:LYS:HG3	3:A:326:LYS:O	2.02	0.58
3:A:27:LYS:HG3	3:A:28:ASN:ND2	2.18	0.58
3:A:292:THR:O	3:A:298:ILE:HA	2.03	0.58
3:A:11:LEU:HD23	3:A:11:LEU:H	1.68	0.58
3:A:203:GLU:O	3:A:205:THR:N	2.37	0.58
3:A:254:ARG:NH1	3:A:255:ILE:N	2.52	0.58
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.32	0.58
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.38	0.58
3:A:133:ASN:O	3:A:137:ARG:HG3	2.04	0.58
3:A:138:ILE:HD12	3:A:228:LEU:HD11	1.86	0.57
3:A:328:ARG:O	3:A:333:ARG:NE	2.26	0.57
3:A:215:VAL:HG12	3:A:219:GLN:OE1	2.04	0.57
3:A:285:HIS:NE2	5:A:574:HOH:O	2.32	0.57
3:A:135:HIS:O	3:A:138:ILE:HB	2.04	0.57
1:T:6:DG:H2"	1:T:7:DA:H8	1.62	0.57
3:A:15:ILE:CB	3:A:46:ILE:HD11	2.35	0.57
3:A:41:LYS:O	3:A:44:SER:HB3	2.04	0.57
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.19	0.57
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.17	0.57
3:A:138:ILE:HD12	3:A:228:LEU:HD12	1.84	0.57
3:A:243:SER:OG	3:A:249:GLU:HG3	2.04	0.57
3:A:41:LYS:HD3	3:A:42:ALA:N	2.20	0.57
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.86	0.57
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.86	0.56
3:A:169:VAL:HG13	3:A:170:ASP:H	1.70	0.56
3:A:35:LYS:O	3:A:38:ALA:HB3	2.04	0.56
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.87	0.56
3:A:16:THR:O	3:A:20:THR:HG23	2.06	0.56
3:A:254:ARG:NH1	3:A:255:ILE:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.86	0.56
3:A:267:CYS:SG	3:A:297:THR:HA	2.46	0.56
3:A:180:SER:HA	3:A:183:ARG:HE	1.70	0.56
3:A:253:ARG:NH1	5:A:503:HOH:O	2.38	0.56
3:A:134:HIS:O	3:A:137:ARG:HB2	2.05	0.56
3:A:243:SER:HB3	3:A:249:GLU:CA	2.26	0.55
1:T:4:DT:H71	5:T:645:HOH:O	2.05	0.55
3:A:19:LEU:HD23	3:A:43:ALA:CB	2.35	0.55
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.42	0.55
3:A:259:LEU:CD1	3:A:260:ILE:H	2.13	0.55
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.37	0.55
3:A:283:ARG:HG2	3:A:293:ILE:HB	1.88	0.55
2:P:1:DT:H2'	2:P:2:DC:C6	2.42	0.55
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.37	0.55
3:A:188:SER:HB3	5:A:522:HOH:O	2.07	0.55
2:P:6:DT:H5'	5:P:561:HOH:O	2.06	0.54
2:P:6:DT:H2'	2:P:7:DG:C8	2.42	0.54
3:A:59:ALA:O	3:A:62:LEU:N	2.32	0.54
3:A:141:LYS:HE2	3:A:142:TYR:OH	2.06	0.54
3:A:169:VAL:HG13	3:A:170:ASP:N	2.22	0.54
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.90	0.54
3:A:103:VAL:HG11	3:A:106:ILE:CD1	2.38	0.54
3:A:288:GLU:C	3:A:290:GLY:H	2.11	0.54
3:A:81:LYS:NZ	3:A:86:GLU:HB2	2.21	0.54
3:A:12:ASN:HA	5:A:549:HOH:O	2.08	0.53
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.55	0.53
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.08	0.53
2:P:5:DA:P	3:A:109:SER:HB3	2.48	0.53
3:A:149:ARG:NH2	3:A:188:SER:HA	2.24	0.53
3:A:195:LEU:HD12	3:A:196:THR:H	1.72	0.53
3:A:267:CYS:O	3:A:270:LEU:HB3	2.08	0.53
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.38	0.53
3:A:121:THR:HG23	3:A:124:ASP:CG	2.29	0.53
3:A:181:PHE:HD1	5:A:530:HOH:O	1.92	0.53
3:A:38:ALA:O	3:A:41:LYS:HD3	2.08	0.53
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.40	0.53
3:A:204:SER:O	3:A:206:LYS:N	2.41	0.53
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.43	0.53
3:A:41:LYS:O	3:A:45:VAL:HG13	2.08	0.52
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.91	0.52
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:19:LEU:HD23	3:A:43:ALA:HA	1.90	0.52
3:A:165:GLU:CB	3:A:217:GLN:HG3	2.28	0.52
3:A:128:ASN:ND2	3:A:128:ASN:N	2.56	0.52
3:A:83:ARG:O	3:A:87:LYS:N	2.38	0.52
3:A:202:SER:N	3:A:261:PRO:HB3	2.24	0.52
3:A:191:MET:O	3:A:191:MET:HG3	2.08	0.52
3:A:235:PHE:CE1	3:A:237:GLY:N	2.77	0.52
3:A:326:LYS:O	3:A:328:ARG:HG2	2.08	0.52
3:A:21:GLU:OE1	3:A:85:LEU:HG	2.09	0.52
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.24	0.52
3:A:228:LEU:HB2	3:A:236:MET:O	2.10	0.52
3:A:240:GLN:NE2	3:A:250:TYR:O	2.43	0.52
3:A:253:ARG:HH11	3:A:253:ARG:HG2	1.75	0.52
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.44	0.52
3:A:155:MET:HE2	3:A:188:SER:HB2	1.90	0.51
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.39	0.51
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.42	0.51
3:A:243:SER:O	3:A:244:LYS:O	2.29	0.51
3:A:15:ILE:CD1	3:A:73:ILE:HG21	2.41	0.51
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.79	0.51
3:A:183:ARG:HH11	3:A:275:SER:HB3	1.76	0.51
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.75	0.51
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.80	0.50
3:A:196:THR:OG1	3:A:262:LYS:HA	2.11	0.50
3:A:164:ASN:O	3:A:168:LYS:HG2	2.12	0.50
2:P:6:DT:C5'	2:P:6:DT:H6	2.24	0.50
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.94	0.50
3:A:29:VAL:HG21	3:A:94:SER:HA	1.94	0.50
3:A:294:ASN:HB2	3:A:295:GLU:OE1	2.12	0.50
3:A:55:SER:O	3:A:58:GLU:HB3	2.12	0.50
2:P:6:DT:H2"	2:P:7:DG:C5'	2.12	0.49
3:A:292:THR:HG22	3:A:299:ARG:O	2.13	0.49
3:A:155:MET:HE3	3:A:188:SER:HB2	1.93	0.49
3:A:192:ASP:N	3:A:192:ASP:OD1	2.46	0.49
3:A:79:THR:O	3:A:79:THR:OG1	2.29	0.49
3:A:294:ASN:ND2	5:A:581:HOH:O	2.44	0.49
1:T:3:DT:H2'	1:T:4:DT:H71	1.95	0.49
3:A:75:GLU:O	3:A:79:THR:HG23	2.13	0.49
3:A:151:PRO:O	3:A:154:GLU:HB2	2.12	0.48
3:A:212:HIS:N	3:A:212:HIS:CD2	2.81	0.48
3:A:127:LYS:HE3	3:A:127:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:171:SER:O	3:A:171:SER:OG	2.30	0.48
3:A:293:ILE:HD12	3:A:293:ILE:HG23	1.56	0.48
3:A:138:ILE:HG21	3:A:228:LEU:HD11	1.95	0.48
3:A:142:TYR:CE1	3:A:252:HIS:CG	3.01	0.48
3:A:259:LEU:O	3:A:260:ILE:HD13	2.14	0.48
3:A:79:THR:O	3:A:81:LYS:N	2.47	0.47
3:A:155:MET:HA	3:A:158:MET:HE3	1.96	0.47
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.77	0.47
3:A:166:VAL:O	3:A:169:VAL:HG12	2.14	0.47
3:A:230:LYS:HE2	3:A:230:LYS:HB3	1.53	0.47
3:A:295:GLU:OE1	3:A:295:GLU:N	2.45	0.47
3:A:265:TYR:O	3:A:268:GLY:N	2.48	0.47
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.50	0.47
3:A:317:LYS:HD2	3:A:321:ASP:OD1	2.15	0.47
3:A:259:LEU:C	3:A:260:ILE:HG12	2.33	0.47
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.44	0.47
3:A:150:ILE:HG12	3:A:253:ARG:HH11	1.80	0.47
3:A:201:THR:HA	3:A:261:PRO:CA	2.45	0.47
3:A:254:ARG:HH11	3:A:255:ILE:H	1.62	0.47
3:A:22:LEU:HG	3:A:39:TYR:CE1	2.50	0.47
3:A:323:ILE:C	3:A:324:GLN:HG2	2.35	0.47
3:A:327:TYR:CD1	3:A:328:ARG:N	2.81	0.47
3:A:79:THR:C	3:A:81:LYS:H	2.19	0.46
3:A:181:PHE:HA	5:A:530:HOH:O	2.14	0.46
3:A:254:ARG:HH11	3:A:255:ILE:N	2.11	0.46
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.80	0.46
3:A:276:ASP:O	3:A:280:LYS:HG3	2.14	0.46
3:A:15:ILE:HD13	3:A:73:ILE:HG21	1.98	0.46
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.65	0.46
3:A:240:GLN:NE2	3:A:252:HIS:CE1	2.84	0.46
3:A:22:LEU:CB	3:A:39:TYR:CE1	2.98	0.46
3:A:149:ARG:NH2	3:A:188:SER:CA	2.78	0.46
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.94	0.46
3:A:174:ILE:HB	3:A:196:THR:HG22	1.98	0.46
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.96	0.46
3:A:284:ALA:O	3:A:287:LEU:HB2	2.15	0.46
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.98	0.46
3:A:241:LEU:CB	3:A:250:TYR:CD2	2.96	0.46
3:A:53:ILE:HG21	3:A:59:ALA:HB2	1.98	0.46
2:P:5:DA:C2'	2:P:6:DT:H71	2.46	0.46
3:A:25:PHE:CD1	3:A:88:ILE:CD1	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.25	0.46
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.51	0.46
3:A:205:THR:HA	5:A:609:HOH:O	2.16	0.46
3:A:303:VAL:O	3:A:305:GLY:N	2.49	0.46
2:P:6:DT:C2'	2:P:7:DG:C8	2.99	0.45
3:A:127:LYS:C	3:A:128:ASN:HD22	2.19	0.45
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.47	0.45
3:A:25:PHE:CD1	3:A:88:ILE:HD13	2.52	0.45
3:A:31:GLN:N	5:A:623:HOH:O	2.28	0.45
3:A:157:GLN:O	3:A:161:ILE:HG13	2.16	0.45
3:A:32:ALA:O	3:A:36:TYR:HB3	2.17	0.45
3:A:28:ASN:ND2	3:A:28:ASN:N	2.55	0.45
3:A:183:ARG:HH11	3:A:275:SER:CB	2.29	0.45
2:P:2:DC:H1'	5:P:617:HOH:O	2.16	0.44
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.99	0.44
3:A:46:ILE:HG22	3:A:62:LEU:HD23	1.99	0.44
3:A:76:PHE:HD2	3:A:77:LEU:HD12	1.82	0.44
3:A:200:PHE:O	3:A:262:LYS:N	2.46	0.44
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.31	0.44
3:A:183:ARG:HE	3:A:183:ARG:HB2	1.51	0.44
3:A:254:ARG:NH1	3:A:254:ARG:CB	2.78	0.44
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.53	0.44
3:A:138:ILE:CD1	3:A:226:ASP:HB3	2.48	0.44
3:A:172:GLU:HG2	3:A:198:PRO:HG2	2.00	0.44
3:A:195:LEU:O	3:A:260:ILE:HB	2.17	0.44
3:A:138:ILE:HD11	3:A:226:ASP:HB3	2.00	0.44
3:A:56:GLY:O	3:A:59:ALA:HB3	2.17	0.44
3:A:140:LEU:HD12	3:A:140:LEU:HA	1.74	0.44
3:A:156:LEU:HD23	3:A:156:LEU:HA	1.67	0.44
3:A:159:GLN:O	3:A:163:LEU:HG	2.18	0.44
2:P:5:DA:P	3:A:107:GLY:HA3	2.57	0.43
3:A:261:PRO:HB2	3:A:263:ASP:OD1	2.17	0.43
3:A:15:ILE:CG2	3:A:46:ILE:HD11	2.48	0.43
3:A:190:ASP:OD1	3:A:190:ASP:O	2.37	0.43
3:A:15:ILE:CG2	3:A:46:ILE:CD1	2.96	0.43
3:A:207:GLN:HB3	3:A:210:LEU:HD12	2.00	0.43
3:A:287:LEU:HD13	3:A:291:PHE:O	2.18	0.43
3:A:191:MET:HA	5:A:502:HOH:O	2.17	0.43
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.47	0.43
2:P:6:DT:H5'	2:P:6:DT:H6	1.82	0.43
3:A:254:ARG:HH11	3:A:254:ARG:CA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.91	0.43
3:A:299:ARG:HG2	3:A:310:PRO:CA	2.49	0.43
3:A:320:PHE:CE1	3:A:328:ARG:HG3	2.54	0.43
3:A:150:ILE:HG23	3:A:253:ARG:NE	2.33	0.43
3:A:309:GLU:O	3:A:311:LEU:HD13	2.19	0.43
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.68	0.43
3:A:261:PRO:O	3:A:264:GLN:N	2.49	0.43
3:A:303:VAL:C	3:A:305:GLY:H	2.22	0.43
3:A:270:LEU:HD21	3:A:282:MET:HE3	1.99	0.42
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.54	0.42
3:A:309:GLU:N	3:A:310:PRO:CD	2.82	0.42
3:A:311:LEU:HA	3:A:311:LEU:HD12	1.78	0.42
3:A:22:LEU:HD22	3:A:85:LEU:HD13	2.01	0.42
3:A:264:GLN:NE2	3:A:296:TYR:HB3	2.35	0.42
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.80	0.42
3:A:62:LEU:HA	3:A:62:LEU:HD12	1.63	0.42
3:A:93:THR:HG22	3:A:94:SER:N	2.30	0.42
3:A:217:GLN:HE22	3:A:220:LYS:HD3	1.83	0.42
3:A:282:MET:HG2	5:A:550:HOH:O	2.19	0.42
3:A:292:THR:O	3:A:298:ILE:HG13	2.20	0.42
3:A:22:LEU:HD22	3:A:85:LEU:CD1	2.49	0.42
3:A:108:PRO:O	3:A:112:ARG:HG3	2.19	0.42
3:A:127:LYS:HD2	3:A:127:LYS:N	2.34	0.42
3:A:211:LEU:HD12	3:A:211:LEU:C	2.39	0.42
3:A:77:LEU:HD12	3:A:77:LEU:HA	1.73	0.42
3:A:151:PRO:O	3:A:154:GLU:N	2.52	0.42
3:A:235:PHE:CE1	3:A:237:GLY:HA3	2.55	0.42
3:A:288:GLU:O	3:A:290:GLY:N	2.53	0.42
3:A:142:TYR:CE1	3:A:252:HIS:CD2	3.08	0.42
3:A:191:MET:HG2	3:A:255:ILE:HG13	2.02	0.42
3:A:286:ALA:HB2	3:A:323:ILE:HG21	2.01	0.42
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.68	0.42
3:A:79:THR:HG23	3:A:79:THR:H	1.47	0.42
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.50	0.42
3:A:217:GLN:NE2	3:A:217:GLN:CA	2.77	0.41
3:A:267:CYS:SG	3:A:297:THR:CA	3.08	0.41
3:A:29:VAL:HG21	3:A:94:SER:OG	2.20	0.41
3:A:101:THR:HA	3:A:106:ILE:HG22	2.02	0.41
3:A:121:THR:HG23	3:A:124:ASP:OD1	2.20	0.41
3:A:29:VAL:CG2	3:A:97:ILE:HD12	2.36	0.41
3:A:270:LEU:HD21	3:A:282:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:260:ILE:HG22	3:A:261:PRO:N	2.36	0.41
3:A:286:ALA:HB1	3:A:293:ILE:HD11	2.02	0.41
3:A:296:TYR:O	3:A:297:THR:HG23	2.20	0.41
3:A:183:ARG:NH1	3:A:275:SER:CB	2.84	0.41
3:A:264:GLN:NE2	3:A:297:THR:HG23	2.35	0.41
3:A:318:ASP:O	3:A:322:TYR:CG	2.74	0.41
3:A:114:PHE:O	3:A:119:ILE:N	2.53	0.41
3:A:329:GLU:O	3:A:333:ARG:HG2	2.21	0.41
3:A:81:LYS:HZ2	3:A:86:GLU:HB2	1.85	0.41
3:A:103:VAL:O	3:A:103:VAL:HG12	2.21	0.41
3:A:150:ILE:N	3:A:188:SER:O	2.48	0.41
3:A:239:CYS:N	3:A:253:ARG:O	2.49	0.41
3:A:264:GLN:HE21	3:A:297:THR:HG23	1.86	0.41
3:A:331:LYS:HG2	3:A:332:ASP:N	2.29	0.41
3:A:29:VAL:HA	3:A:97:ILE:HD12	2.03	0.41
3:A:241:LEU:HB2	3:A:250:TYR:CG	2.55	0.41
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.85	0.40
3:A:244:LYS:H	3:A:244:LYS:HG2	1.62	0.40
3:A:33:ILE:O	3:A:36:TYR:HD2	2.04	0.40
3:A:102:ARG:H	3:A:102:ARG:HG3	1.76	0.40
3:A:155:MET:HB3	3:A:181:PHE:CD1	2.56	0.40
3:A:206:LYS:O	3:A:207:GLN:HB2	2.21	0.40
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.44	0.40
3:A:253:ARG:NH1	3:A:253:ARG:CG	2.79	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%)	268 (82%)	39 (12%)	18 (6%)	2 20

All (18) 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	289	LYS
3	A	295	GLU
3	A	298	ILE
3	A	80	GLY
3	A	91	ASP
3	A	185	ALA
3	A	207	GLN
3	A	304	THR
3	A	10	THR
3	A	13	GLY
3	A	309	GLU
3	A	310	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	231 (80%)	57 (20%)	1 8

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	18	MET
3	A	22	LEU
3	A	30	SER
3	A	33	ILE
3	A	36	TYR
3	A	37	ASN

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Mol	Chain	Res	Type
3	A	41	LYS
3	A	44	SER
3	A	45	VAL
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	79	THR
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
3	A	128	ASN
3	A	133	ASN
3	A	138	ILE
3	A	145	ASP
3	A	153	GLU
3	A	171	SER
3	A	182	ARG
3	A	191	MET
3	A	192	ASP
3	A	198	PRO
3	A	201	THR
3	A	203	GLU
3	A	214	VAL
3	A	218	LEU
3	A	229	SER
3	A	230	LYS
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	258	ARG
3	A	259	LEU
3	A	263	ASP
3	A	277	ILE
3	A	287	LEU
3	A	294	ASN
3	A	301	LEU
3	A	304	THR

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Mol	Chain	Res	Type
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	324	GLN
3	A	325	TRP
3	A	327	TYR
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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	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 2 ligands modelled in this entry, 2 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)

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	T	8/8 (100%)	-0.93	0	100	100	16, 30, 73, 93	0
2	P	7/7 (100%)	-1.26	0	100	100	11, 26, 50, 64	0
3	A	325/335 (97%)	-1.20	0	100	100	1, 32, 86, 98	0
All	All	340/350 (97%)	-1.20	0	100	100	1, 33, 86, 98	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
4	CR	A	340	1/1	0.93	0.14	67,67,67,67	0
4	CR	A	341	1/1	0.99	0.06	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.