



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:00 AM GMT

PDB ID : 7ICM
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SIX BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF MNCL2 (1.0 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

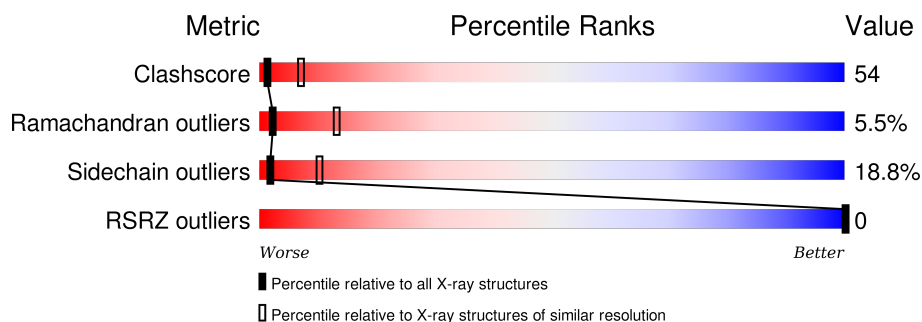
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	T	7	
2	P	6	
3	A	335	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3027 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*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	7	Total	C	N	O	P	0	0	0
			122	58	20	38	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	P	0	0	0
			126	59	25	36	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	26	0	0
			2623	1657	458	499	9			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

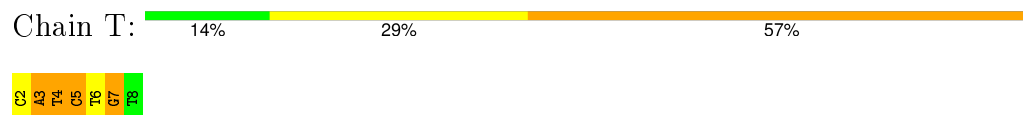
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		
5	P	20	Total	O	0	0
			20	20		
5	T	12	Total	O	0	0
			12	12		

3 Residue-property plots [i](#)

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

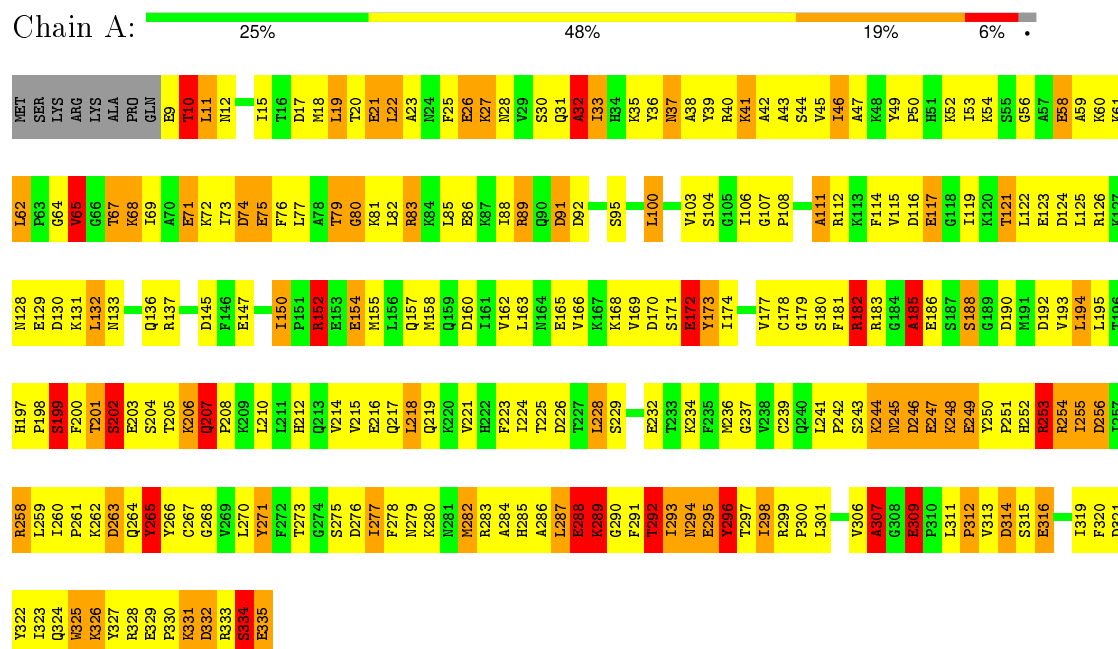
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.47Å 57.76Å 48.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 11.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.00) 90.7 (11.95-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.70Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.152 , (Not available) 0.148 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 131.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 12947 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3027	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NA

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	2.40	6/135 (4.4%)	2.48	12/207 (5.8%)
2	P	2.71	8/141 (5.7%)	3.05	17/214 (7.9%)
3	A	1.26	26/2672 (1.0%)	1.74	63/3590 (1.8%)
All	All	1.43	40/2948 (1.4%)	1.87	92/4011 (2.3%)

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
3	A	2	0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DT	C1'-N1	13.94	1.67	1.49
3	A	58	GLU	CD-OE1	8.87	1.35	1.25
2	P	5	DT	N1-C2	8.43	1.44	1.38
2	P	6	DG	C3'-O3'	-8.26	1.33	1.44
1	T	7	DG	C3'-O3'	-8.04	1.33	1.44
3	A	147	GLU	CD-OE2	7.59	1.33	1.25
3	A	75	GLU	CD-OE1	7.56	1.33	1.25
2	P	3	DG	C5-C6	-7.50	1.34	1.42
2	P	5	DT	C3'-O3'	-7.49	1.34	1.44
3	A	203	GLU	CD-OE1	7.28	1.33	1.25
2	P	1	DC	N1-C6	-7.22	1.32	1.37
3	A	26	GLU	CD-OE1	7.07	1.33	1.25
3	A	86	GLU	CD-OE1	7.05	1.33	1.25
1	T	3	DA	N9-C4	6.95	1.42	1.37
3	A	309	GLU	CD-OE2	6.92	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	6	DG	N9-C4	-6.88	1.32	1.38
3	A	249	GLU	CD-OE2	6.85	1.33	1.25
3	A	71	GLU	CD-OE1	6.65	1.32	1.25
3	A	295	GLU	CD-OE1	6.46	1.32	1.25
3	A	186	GLU	CD-OE1	6.39	1.32	1.25
3	A	129	GLU	CD-OE1	6.39	1.32	1.25
3	A	172	GLU	CD-OE2	6.38	1.32	1.25
3	A	232	GLU	CD-OE2	6.32	1.32	1.25
3	A	165	GLU	CD-OE2	6.30	1.32	1.25
1	T	5	DC	C1'-N1	6.29	1.57	1.49
3	A	329	GLU	CD-OE2	6.28	1.32	1.25
1	T	4	DT	N1-C2	6.12	1.43	1.38
3	A	21	GLU	CD-OE1	6.10	1.32	1.25
1	T	7	DG	N9-C4	-6.08	1.33	1.38
3	A	117	GLU	CD-OE2	6.07	1.32	1.25
3	A	216	GLU	CD-OE2	6.00	1.32	1.25
3	A	123	GLU	CD-OE1	5.82	1.32	1.25
3	A	335	GLU	CD-OE2	5.73	1.31	1.25
3	A	316	GLU	CD-OE2	5.72	1.31	1.25
3	A	288	GLU	CD-OE2	5.70	1.31	1.25
1	T	7	DG	C1'-N9	-5.60	1.39	1.47
2	P	3	DG	C6-N1	-5.33	1.35	1.39
3	A	9	GLU	CD-OE2	5.28	1.31	1.25
3	A	247	GLU	CD-OE1	5.22	1.31	1.25
3	A	154	GLU	CD-OE2	5.15	1.31	1.25

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DC	P-O3'-C3'	12.82	135.08	119.70
2	P	2	DA	O4'-C4'-C3'	-11.18	99.29	106.00
2	P	5	DT	C2-N1-C1'	10.41	134.85	118.20
2	P	4	DA	O4'-C1'-N9	-10.28	100.80	108.00
2	P	5	DT	C6-N1-C1'	-10.04	105.34	120.40
3	A	271	TYR	CB-CG-CD1	-9.38	115.37	121.00
1	T	4	DT	C6-N1-C1'	-8.99	106.92	120.40
3	A	192	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	T	7	DG	P-O3'-C3'	-8.77	109.18	119.70
1	T	4	DT	C2-N1-C1'	8.32	131.51	118.20
2	P	2	DA	C4'-C3'-C2'	-7.81	96.07	103.10
3	A	89	ARG	NE-CZ-NH1	7.67	124.14	120.30
2	P	1	DC	C6-N1-C1'	-7.65	111.62	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	74	ASP	CB-CG-OD1	7.64	125.18	118.30
3	A	92	ASP	CB-CG-OD2	-7.53	111.52	118.30
3	A	332	ASP	CB-CG-OD1	-7.45	111.59	118.30
2	P	1	DC	C2-N1-C1'	7.41	126.95	118.80
2	P	5	DT	P-O5'-C5'	-7.32	109.18	120.90
3	A	263	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	T	3	DA	O4'-C1'-N9	-7.21	102.95	108.00
3	A	130	ASP	CB-CG-OD2	-7.21	111.81	118.30
3	A	253	ARG	NE-CZ-NH1	7.16	123.88	120.30
2	P	2	DA	P-O5'-C5'	-7.16	109.44	120.90
3	A	182	ARG	NE-CZ-NH1	7.13	123.87	120.30
3	A	182	ARG	NE-CZ-NH2	-7.02	116.79	120.30
3	A	173	TYR	CB-CG-CD1	-6.99	116.81	121.00
2	P	4	DA	P-O3'-C3'	6.97	128.07	119.70
3	A	170	ASP	CB-CG-OD1	6.89	124.50	118.30
3	A	292	THR	N-CA-CB	6.84	123.30	110.30
3	A	253	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	A	266	TYR	CA-CB-CG	-6.81	100.45	113.40
3	A	314	ASP	CB-CG-OD1	-6.79	112.19	118.30
3	A	185	ALA	N-CA-CB	6.78	119.59	110.10
3	A	116	ASP	CB-CG-OD2	-6.75	112.22	118.30
3	A	190	ASP	CB-CG-OD1	6.71	124.33	118.30
3	A	263	ASP	CB-CG-OD1	6.63	124.26	118.30
3	A	199	SER	N-CA-CB	-6.47	100.79	110.50
3	A	183	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	P	5	DT	N3-C2-O2	-6.44	118.43	122.30
2	P	6	DG	C4-N9-C1'	-6.43	118.14	126.50
3	A	265	TYR	CB-CG-CD1	-6.32	117.21	121.00
3	A	190	ASP	CB-CG-OD2	-6.27	112.66	118.30
3	A	17	ASP	CB-CG-OD1	-6.12	112.79	118.30
3	A	86	GLU	CB-CA-C	6.09	122.58	110.40
2	P	3	DG	P-O3'-C3'	6.08	127.00	119.70
3	A	241	LEU	C-N-CD	-5.98	107.44	120.60
3	A	271	TYR	CA-CB-CG	-5.96	102.08	113.40
3	A	202	SER	N-CA-CB	-5.95	101.57	110.50
3	A	326	LYS	CD-CE-NZ	5.88	125.21	111.70
3	A	152	ARG	N-CA-CB	5.87	121.17	110.60
3	A	92	ASP	CB-CG-OD1	5.80	123.53	118.30
3	A	74	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	T	2	DC	C2-N1-C1'	5.75	125.13	118.80
3	A	332	ASP	CB-CG-OD2	5.75	123.48	118.30
1	T	7	DG	C4-N9-C1'	-5.74	119.04	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	91	ASP	CB-CG-OD1	-5.71	113.16	118.30
3	A	126	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	P	6	DG	C8-N9-C1'	5.67	134.37	127.00
3	A	32	ALA	N-CA-C	5.64	126.24	111.00
3	A	246	ASP	CB-CG-OD1	-5.60	113.26	118.30
3	A	296	TYR	CB-CA-C	-5.60	99.20	110.40
3	A	313	VAL	CB-CA-C	-5.60	100.76	111.40
1	T	5	DC	P-O3'-C3'	5.57	126.38	119.70
1	T	6	DT	C6-N1-C1'	-5.55	112.07	120.40
1	T	3	DA	C2-N3-C4	5.51	113.35	110.60
3	A	173	TYR	CB-CG-CD2	5.49	124.29	121.00
3	A	334	SER	CB-CA-C	5.49	120.52	110.10
3	A	111	ALA	N-CA-CB	5.47	117.76	110.10
3	A	65	VAL	CA-CB-CG2	-5.46	102.72	110.90
3	A	130	ASP	CB-CG-OD1	5.45	123.21	118.30
3	A	92	ASP	N-CA-CB	5.45	120.41	110.60
3	A	276	ASP	CB-CG-OD2	-5.39	113.45	118.30
3	A	170	ASP	CB-CG-OD2	-5.38	113.45	118.30
3	A	335	GLU	N-CA-CB	5.36	120.24	110.60
3	A	254	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	A	265	TYR	CB-CG-CD2	5.34	124.20	121.00
3	A	168	LYS	N-CA-CB	5.33	120.19	110.60
1	T	3	DA	N9-C1'-C2'	5.31	122.68	112.60
3	A	246	ASP	CB-CG-OD2	5.29	123.06	118.30
3	A	86	GLU	N-CA-CB	5.26	120.08	110.60
3	A	307	ALA	N-CA-CB	5.25	117.45	110.10
2	P	5	DT	O5'-P-OP1	-5.24	100.98	105.70
3	A	256	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	T	2	DC	C6-N1-C1'	-5.22	114.54	120.80
3	A	20	THR	N-CA-CB	5.21	120.19	110.30
3	A	225	THR	CA-CB-CG2	-5.13	105.22	112.40
3	A	83	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	T	5	DC	N3-C4-C5	-5.08	119.87	121.90
2	P	5	DT	P-O3'-C3'	5.08	125.80	119.70
3	A	126	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	A	201	THR	CA-CB-CG2	-5.07	105.30	112.40
3	A	91	ASP	CB-CG-OD2	5.03	122.83	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	32	ALA	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	A	40	ARG	CA

There are no planarity outliers.

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	T	122	0	69	3	0
2	P	126	0	68	6	0
3	A	2623	0	2641	292	2
4	A	2	0	0	0	0
5	A	122	0	0	11	0
5	P	20	0	0	0	0
5	T	12	0	0	3	0
All	All	3027	0	2778	300	2

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 54.

All (300) 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:23:ALA:HB2	3:A:39:TYR:HB2	1.23	1.08
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.34	1.06
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.43	0.98
3:A:245:ASN:H	3:A:245:ASN:HD22	1.01	0.94
3:A:245:ASN:N	3:A:245:ASN:HD22	1.64	0.94
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.04	0.93
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.49	0.91
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.53	0.90
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.54	0.89
2:P:1:DC:H2''	2:P:2:DA:H5''	1.54	0.89
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.56	0.88
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.56	0.87
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.40	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.58	0.85
2:P:1:DC:C2'	2:P:2:DA:H5''	2.07	0.84
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.06	0.83
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.10	0.82
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.63	0.81
3:A:33:ILE:O	3:A:37:ASN:HB2	1.81	0.80
3:A:12:ASN:HD21	3:A:53:ILE:H	1.29	0.80
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.80	0.79
3:A:11:LEU:HD23	3:A:11:LEU:H	1.47	0.79
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.63	0.79
3:A:162:VAL:O	3:A:166:VAL:HG23	1.82	0.79
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.63	0.79
3:A:207:GLN:O	3:A:210:LEU:HB2	1.83	0.78
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.83	0.78
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.80	0.78
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.18	0.77
3:A:245:ASN:H	3:A:245:ASN:ND2	1.81	0.76
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.15	0.75
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.16	0.75
3:A:154:GLU:O	3:A:158:MET:HG3	1.87	0.73
3:A:59:ALA:O	3:A:62:LEU:HB2	1.89	0.73
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.69	0.73
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.18	0.73
3:A:294:ASN:HB2	3:A:295:GLU:OE2	1.89	0.72
3:A:155:MET:HA	3:A:158:MET:HE3	1.71	0.72
3:A:41:LYS:HD3	3:A:42:ALA:N	2.05	0.72
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.19	0.72
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.36	0.71
3:A:282:MET:HG2	5:A:555:HOH:O	1.90	0.71
3:A:18:MET:HE3	3:A:76:PHE:CD2	2.25	0.71
3:A:278:PHE:HB2	3:A:333:ARG:O	1.91	0.70
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.12	0.70
3:A:245:ASN:N	3:A:245:ASN:ND2	2.39	0.68
3:A:152:ARG:HA	3:A:155:MET:HB2	1.75	0.68
3:A:179:GLY:O	3:A:182:ARG:HB3	1.94	0.67
3:A:80:GLY:O	3:A:81:LYS:HG2	1.94	0.67
3:A:166:VAL:O	3:A:169:VAL:HG12	1.93	0.67
3:A:306:VAL:HG23	3:A:307:ALA:N	2.09	0.67
3:A:68:LYS:O	3:A:72:LYS:HE3	1.95	0.67
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.31	0.66
3:A:243:SER:HB3	3:A:249:GLU:HA	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:69:ILE:O	3:A:73:ILE:HG13	1.96	0.66
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.11	0.66
3:A:121:THR:O	3:A:124:ASP:HB2	1.95	0.65
3:A:58:GLU:O	3:A:61:LYS:HB2	1.96	0.65
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.78	0.65
3:A:18:MET:CE	3:A:76:PHE:HB2	2.27	0.65
3:A:201:THR:HA	3:A:261:PRO:CB	2.27	0.65
3:A:31:GLN:N	5:A:641:HOH:O	2.27	0.65
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.33	0.64
3:A:270:LEU:HD21	3:A:282:MET:CE	2.28	0.64
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.10	0.64
3:A:178:CYS:HA	3:A:182:ARG:HD3	1.80	0.64
3:A:217:GLN:O	3:A:221:VAL:HG22	1.98	0.63
3:A:124:ASP:O	3:A:128:ASN:ND2	2.31	0.63
3:A:331:LYS:HD2	3:A:332:ASP:N	2.14	0.63
3:A:262:LYS:HG3	3:A:262:LYS:O	1.98	0.63
3:A:155:MET:HA	3:A:158:MET:CE	2.29	0.63
3:A:271:TYR:HB2	5:A:592:HOH:O	1.98	0.63
3:A:279:ASN:O	3:A:283:ARG:N	2.30	0.62
3:A:201:THR:CG2	3:A:204:SER:HB3	2.30	0.62
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.82	0.62
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.12	0.62
3:A:44:SER:O	3:A:47:ALA:HB3	1.99	0.62
3:A:197:HIS:ND1	3:A:199:SER:HB3	2.15	0.61
3:A:201:THR:HA	3:A:261:PRO:HB3	1.81	0.61
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.15	0.61
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.35	0.61
3:A:12:ASN:ND2	3:A:53:ILE:H	1.96	0.61
3:A:11:LEU:CD2	3:A:11:LEU:H	2.13	0.61
1:T:3:DA:H2"	5:T:573:HOH:O	2.00	0.60
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.01	0.60
3:A:35:LYS:O	3:A:38:ALA:HB3	2.01	0.60
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.42	0.60
3:A:18:MET:HE3	3:A:76:PHE:CG	2.37	0.60
3:A:27:LYS:HG3	3:A:28:ASN:N	2.11	0.59
3:A:236:MET:HG2	3:A:254:ARG:HH22	1.68	0.59
3:A:41:LYS:O	3:A:45:VAL:HG13	2.03	0.59
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.44	0.58
3:A:155:MET:CE	3:A:188:SER:HB2	2.34	0.58
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.38	0.58
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:41:LYS:HD3	3:A:42:ALA:H	1.67	0.57
3:A:166:VAL:HG12	3:A:173:TYR:CB	2.34	0.57
3:A:111:ALA:O	3:A:115:VAL:HG23	2.04	0.57
3:A:207:GLN:OE1	3:A:210:LEU:HG	2.05	0.57
3:A:298:ILE:HG21	3:A:322:TYR:HD2	1.69	0.57
3:A:200:PHE:HB2	5:A:625:HOH:O	2.05	0.57
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.25	0.57
3:A:75:GLU:O	3:A:79:THR:HG23	2.04	0.56
3:A:79:THR:O	3:A:81:LYS:N	2.37	0.56
3:A:155:MET:HE3	3:A:188:SER:HB2	1.88	0.56
3:A:43:ALA:O	3:A:47:ALA:HB2	2.05	0.56
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.41	0.56
3:A:253:ARG:HG2	3:A:253:ARG:HH11	1.68	0.56
3:A:133:ASN:O	3:A:137:ARG:HG3	2.06	0.56
3:A:23:ALA:O	3:A:36:TYR:HD1	1.89	0.56
3:A:36:TYR:CD2	3:A:37:ASN:N	2.74	0.56
3:A:248:LYS:HG2	3:A:248:LYS:O	2.04	0.56
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.88	0.55
3:A:201:THR:HG22	3:A:204:SER:HB3	1.88	0.55
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.72	0.55
3:A:288:GLU:C	3:A:290:GLY:H	2.10	0.55
3:A:264:GLN:HA	5:A:536:HOH:O	2.06	0.55
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.42	0.55
3:A:132:LEU:HB2	3:A:137:ARG:HG2	1.89	0.55
3:A:180:SER:HB2	3:A:185:ALA:HB3	1.89	0.55
3:A:280:LYS:O	3:A:283:ARG:N	2.39	0.55
3:A:315:SER:OG	3:A:316:GLU:N	2.40	0.55
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.88	0.54
1:T:4:DT:H2''	1:T:5:DC:O5'	2.07	0.54
3:A:286:ALA:O	3:A:291:PHE:HB2	2.07	0.54
3:A:212:HIS:HB3	5:A:541:HOH:O	2.07	0.54
3:A:286:ALA:O	3:A:291:PHE:N	2.41	0.54
3:A:319:ILE:O	3:A:322:TYR:HB2	2.08	0.54
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.54	0.54
3:A:321:ASP:O	3:A:324:GLN:N	2.37	0.53
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.44	0.53
2:P:2:DA:C8	2:P:2:DA:H5'	2.44	0.53
3:A:56:GLY:O	3:A:59:ALA:N	2.42	0.53
3:A:114:PHE:CD1	3:A:119:ILE:HD12	2.44	0.53
3:A:15:ILE:HG22	3:A:19:LEU:HD22	1.91	0.53
3:A:299:ARG:HB3	3:A:300:PRO:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:295:GLU:H	3:A:295:GLU:CD	2.13	0.53
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.74	0.52
3:A:202:SER:HB2	3:A:263:ASP:OD1	2.09	0.52
3:A:27:LYS:HG3	3:A:28:ASN:HD22	1.74	0.52
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.92	0.52
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.38	0.52
3:A:18:MET:O	3:A:21:GLU:HB2	2.08	0.52
3:A:108:PRO:O	3:A:112:ARG:HG3	2.09	0.52
3:A:195:LEU:O	3:A:260:ILE:N	2.41	0.52
3:A:237:GLY:O	3:A:254:ARG:NH1	2.43	0.52
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.25	0.52
3:A:157:GLN:HE22	3:A:244:LYS:NZ	2.08	0.52
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.16	0.52
3:A:133:ASN:H	3:A:136:GLN:NE2	2.07	0.52
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.32	0.51
2:P:5:DT:H2''	2:P:6:DG:H5'	1.91	0.51
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.45	0.51
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.26	0.51
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.91	0.51
3:A:267:CYS:SG	3:A:297:THR:HA	2.50	0.51
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.18	0.51
3:A:15:ILE:HG12	3:A:73:ILE:HG23	1.93	0.51
3:A:60:LYS:HE2	3:A:67:THR:HA	1.91	0.51
3:A:18:MET:O	3:A:22:LEU:HD22	2.11	0.51
3:A:300:PRO:HD3	3:A:309:GLU:O	2.11	0.51
3:A:243:SER:CB	3:A:249:GLU:HA	2.42	0.51
3:A:242:PRO:HG2	5:A:589:HOH:O	2.10	0.50
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.46	0.50
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.76	0.50
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.93	0.50
3:A:288:GLU:OE1	3:A:288:GLU:HA	2.01	0.50
3:A:327:TYR:CD1	3:A:328:ARG:N	2.79	0.50
3:A:292:THR:C	3:A:293:ILE:HD13	2.32	0.50
3:A:244:LYS:HB2	3:A:245:ASN:HD22	1.76	0.50
3:A:300:PRO:HG3	3:A:311:LEU:HD11	1.94	0.49
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.42	0.49
3:A:327:TYR:HE1	3:A:333:ARG:NH2	2.09	0.49
3:A:255:ILE:HG12	3:A:256:ASP:N	2.25	0.49
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.12	0.49
3:A:326:LYS:HE2	3:A:328:ARG:HE	1.76	0.49
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.11	0.49
3:A:330:PRO:CA	3:A:333:ARG:HG3	2.40	0.49
3:A:79:THR:C	3:A:81:LYS:H	2.15	0.49
3:A:145:ASP:CG	3:A:252:HIS:H	2.16	0.49
3:A:18:MET:HG2	3:A:22:LEU:CD2	2.43	0.48
3:A:132:LEU:HB3	3:A:136:GLN:HB3	1.95	0.48
3:A:202:SER:HB2	3:A:263:ASP:CG	2.34	0.48
3:A:10:THR:O	3:A:10:THR:HG23	2.10	0.48
3:A:298:ILE:HG23	3:A:311:LEU:HB2	1.95	0.48
3:A:201:THR:HG23	3:A:204:SER:HB3	1.95	0.48
3:A:204:SER:OG	3:A:204:SER:O	2.30	0.48
3:A:275:SER:OG	3:A:277:ILE:HG12	2.14	0.48
3:A:298:ILE:HG21	3:A:322:TYR:CD2	2.47	0.48
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.27	0.48
3:A:312:PRO:O	3:A:322:TYR:OH	2.30	0.48
3:A:250:TYR:HB3	3:A:251:PRO:HD2	1.95	0.48
3:A:229:SER:OG	3:A:236:MET:HB2	2.14	0.48
3:A:132:LEU:HD23	3:A:132:LEU:N	2.28	0.48
3:A:259:LEU:C	3:A:260:ILE:HG12	2.33	0.47
3:A:286:ALA:HB1	3:A:293:ILE:CD1	2.29	0.47
3:A:39:TYR:O	3:A:42:ALA:HB3	2.14	0.47
3:A:265:TYR:O	3:A:268:GLY:N	2.46	0.47
3:A:12:ASN:HA	5:A:642:HOH:O	2.14	0.47
3:A:289:LYS:HD3	3:A:289:LYS:HA	1.64	0.47
3:A:228:LEU:HB2	3:A:236:MET:O	2.14	0.47
3:A:208:PRO:O	3:A:212:HIS:HD2	1.98	0.47
3:A:259:LEU:O	3:A:260:ILE:HD13	2.14	0.47
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.97	0.47
3:A:197:HIS:CG	3:A:198:PRO:CD	2.99	0.46
3:A:166:VAL:CG1	3:A:173:TYR:HB3	2.45	0.46
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.45	0.46
3:A:76:PHE:HD1	3:A:77:LEU:HD12	1.81	0.46
3:A:286:ALA:HB2	3:A:323:ILE:HD13	1.98	0.46
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.58	0.46
3:A:68:LYS:NZ	3:A:68:LYS:CB	2.79	0.46
3:A:293:ILE:HD12	3:A:298:ILE:CG1	2.38	0.46
3:A:205:THR:O	3:A:206:LYS:O	2.33	0.46
3:A:172:GLU:HG2	3:A:198:PRO:CG	2.34	0.46
3:A:152:ARG:NH2	3:A:181:PHE:O	2.49	0.46
3:A:198:PRO:C	3:A:200:PHE:H	2.19	0.46
2:P:5:DT:P	3:A:107:GLY:HA3	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:254:ARG:HH11	3:A:255:ILE:H	1.63	0.46
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.98	0.45
3:A:280:LYS:O	3:A:284:ALA:N	2.45	0.45
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.97	0.45
3:A:288:GLU:O	3:A:290:GLY:N	2.50	0.45
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.46	0.45
3:A:282:MET:SD	3:A:320:PHE:CE1	3.09	0.45
3:A:215:VAL:O	3:A:219:GLN:HG3	2.16	0.45
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.98	0.45
3:A:292:THR:O	3:A:298:ILE:HA	2.15	0.45
3:A:157:GLN:O	3:A:160:ASP:HB3	2.17	0.45
3:A:115:VAL:HG12	3:A:115:VAL:O	2.15	0.45
3:A:221:VAL:HG22	3:A:221:VAL:H	1.48	0.45
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.80	0.45
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.57	0.45
3:A:41:LYS:CD	3:A:42:ALA:N	2.79	0.45
3:A:320:PHE:CD1	3:A:325:TRP:HE3	2.35	0.44
3:A:264:GLN:HB3	5:A:536:HOH:O	2.17	0.44
5:T:617:HOH:O	3:A:234:LYS:HD3	2.17	0.44
3:A:177:VAL:HG22	3:A:193:VAL:HG22	2.00	0.44
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.65	0.44
3:A:32:ALA:O	3:A:36:TYR:HB3	2.18	0.44
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.05	0.44
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.54	0.44
3:A:254:ARG:NH1	3:A:255:ILE:H	2.16	0.44
3:A:104:SER:N	5:A:600:HOH:O	2.30	0.44
3:A:163:LEU:HD23	3:A:163:LEU:HA	1.64	0.44
3:A:255:ILE:HG23	3:A:255:ILE:O	2.17	0.44
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.58	0.44
3:A:287:LEU:HA	3:A:291:PHE:O	2.17	0.44
3:A:182:ARG:NH1	3:A:182:ARG:CG	2.78	0.43
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.68	0.43
3:A:244:LYS:CB	3:A:245:ASN:ND2	2.79	0.43
3:A:100:LEU:CD1	3:A:100:LEU:N	2.79	0.43
2:P:2:DA:H5'	2:P:2:DA:H2'	1.55	0.43
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.32	0.43
3:A:132:LEU:HB2	3:A:137:ARG:CG	2.48	0.43
3:A:260:ILE:HD12	3:A:260:ILE:HG23	1.64	0.43
3:A:150:ILE:HD13	3:A:253:ARG:HG2	2.00	0.43
3:A:28:ASN:HD22	3:A:28:ASN:N	2.17	0.42
3:A:292:THR:O	3:A:293:ILE:HD13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:11:LEU:N	3:A:11:LEU:CD2	2.78	0.42
3:A:37:ASN:HA	3:A:37:ASN:HD22	1.64	0.42
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.54	0.42
3:A:145:ASP:HB3	3:A:252:HIS:H	1.84	0.42
3:A:226:ASP:N	3:A:226:ASP:OD1	2.52	0.42
3:A:18:MET:CE	3:A:76:PHE:CD2	2.99	0.42
1:T:7:DG:N3	5:T:634:HOH:O	2.36	0.42
3:A:210:LEU:HA	3:A:210:LEU:HD23	1.92	0.42
3:A:60:LYS:HE2	3:A:67:THR:CA	2.50	0.42
3:A:264:GLN:HE21	3:A:264:GLN:HB3	1.49	0.42
3:A:85:LEU:CD2	3:A:89:ARG:HH21	2.32	0.42
3:A:289:LYS:HG3	3:A:323:ILE:O	2.20	0.41
3:A:145:ASP:HB3	3:A:252:HIS:O	2.20	0.41
3:A:114:PHE:HB3	3:A:119:ILE:HB	2.01	0.41
3:A:332:ASP:C	3:A:334:SER:H	2.22	0.41
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.55	0.41
3:A:82:LEU:HD23	3:A:85:LEU:HD13	2.01	0.41
3:A:173:TYR:O	3:A:174:ILE:HG12	2.21	0.41
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.87	0.41
3:A:197:HIS:HA	3:A:198:PRO:HD3	1.90	0.41
3:A:201:THR:O	3:A:204:SER:N	2.54	0.41
3:A:18:MET:HG2	3:A:19:LEU:N	2.30	0.41
3:A:68:LYS:O	3:A:71:GLU:HB3	2.21	0.41
3:A:155:MET:CE	3:A:188:SER:CB	2.99	0.41
3:A:223:PHE:CE2	3:A:239:CYS:HB2	2.56	0.41
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.41	0.41
3:A:200:PHE:O	3:A:262:LYS:N	2.44	0.41
3:A:293:ILE:CD1	3:A:298:ILE:CG1	2.99	0.41
3:A:254:ARG:NH1	3:A:255:ILE:N	2.69	0.41
3:A:254:ARG:HH11	3:A:255:ILE:N	2.19	0.41
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.69	0.41
3:A:22:LEU:HA	3:A:22:LEU:HD13	1.79	0.40
3:A:297:THR:HB	5:A:626:HOH:O	2.21	0.40
3:A:27:LYS:CG	3:A:28:ASN:N	2.82	0.40
3:A:49:TYR:HA	3:A:50:PRO:HD3	1.49	0.40
3:A:270:LEU:HD21	3:A:282:MET:HE2	2.03	0.40
3:A:74:ASP:O	3:A:77:LEU:N	2.54	0.40
3:A:223:PHE:CE2	3:A:239:CYS:CB	3.04	0.40
3:A:155:MET:HE3	3:A:188:SER:CB	2.51	0.40
3:A:236:MET:HG2	3:A:254:ARG:NH2	2.35	0.40
3:A:214:VAL:HG22	3:A:215:VAL:N	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:ARG:NH1	3:A:117:GLU:CB[3_558]	1.68	0.52
3:A:83:ARG:NH1	3:A:117:GLU:CA[3_558]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	325/335 (97%)	268 (82%)	39 (12%)	18 (6%)	2	13

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	206	LYS
3	A	244	LYS
3	A	247	GLU
3	A	289	LYS
3	A	307	ALA
3	A	10	THR
3	A	246	ASP
3	A	309	GLU
3	A	334	SER
3	A	91	ASP
3	A	265	TYR
3	A	199	SER
3	A	207	GLN
3	A	80	GLY
3	A	312	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288 / 295 (98%)	234 (81%)	54 (19%)	2 10

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	19	LEU
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	79	THR
3	A	95	SER
3	A	100	LEU
3	A	121	THR
3	A	122	LEU
3	A	131	LYS
3	A	132	LEU
3	A	150	ILE
3	A	152	ARG
3	A	171	SER
3	A	172	GLU
3	A	182	ARG
3	A	188	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	194	LEU
3	A	202	SER
3	A	207	GLN
3	A	218	LEU
3	A	228	LEU
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	277	ILE
3	A	282	MET
3	A	287	LEU
3	A	288	GLU
3	A	289	LYS
3	A	292	THR
3	A	293	ILE
3	A	294	ASN
3	A	296	TYR
3	A	298	ILE
3	A	309	GLU
3	A	314	ASP
3	A	325	TRP
3	A	331	LYS

Some 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	90	GLN
3	A	98	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	222	HIS
3	A	245	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	264	GLN
3	A	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	7/7 (100%)	-1.28	0 100 100	21, 38, 64, 94	0
2	P	6/6 (100%)	-1.41	0 100 100	19, 29, 31, 37	0
3	A	324/335 (96%)	-1.20	0 100 100	7, 36, 84, 100	0
All	All	337/348 (96%)	-1.20	0 100 100	7, 36, 84, 100	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NA	A	342	1/1	0.94	0.13	1.39	38,38,38,38	0
4	NA	A	341	1/1	0.99	0.09	0.44	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.