



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:53 pm BST

PDB ID : 9ICJ
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-15
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

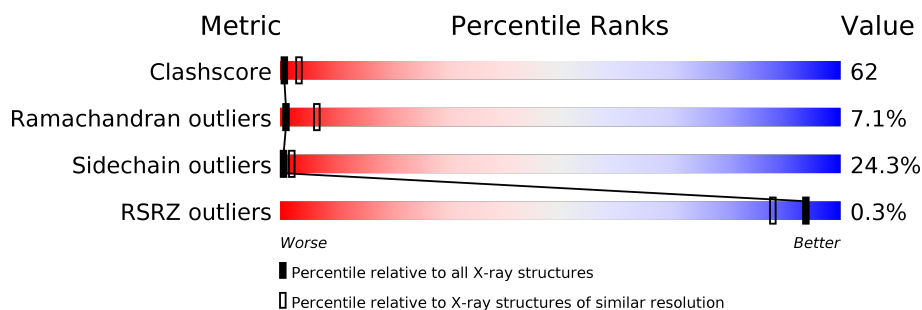
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	8	
2	P	7	
3	A	335	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3056 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
1	T	8	Total	C	N	O	P	0	0	0
			145	69	27	42	7			

- 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
2	P	7	Total	C	N	O	P	0	0	0
			144	69	24	44	7			

- 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	9	0	0
			2623	1657	458	499	9			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	15	Total O 15 15	0	0
6	P	18	Total O 18 18	0	0
6	A	104	Total O 104 104	0	0

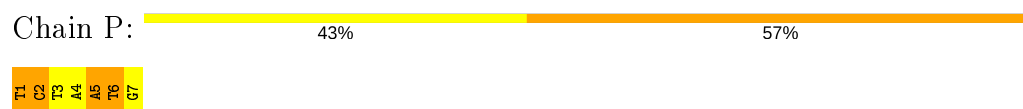
3 Residue-property plots

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

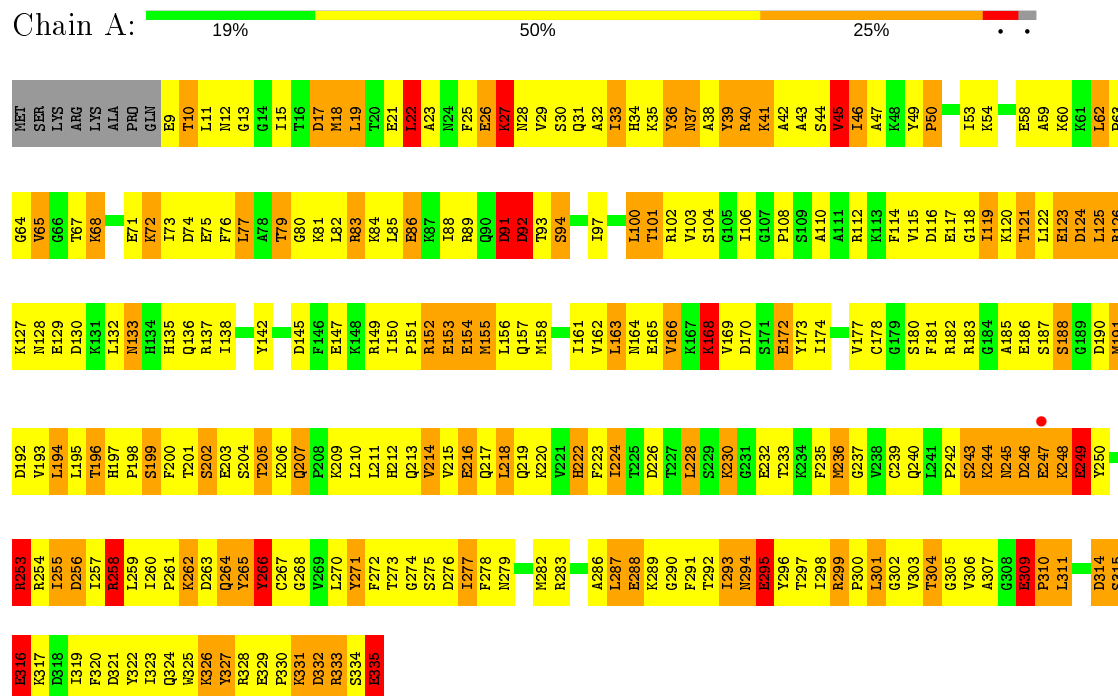
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*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	179.76 Å 57.73 Å 48.38 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 15.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.0 (20.00-3.10) 82.7 (15.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.82 Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.149 , (Not available) 0.143 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 232.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3056	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	T	2.17	4/162 (2.5%)	3.32	25/249 (10.0%)
2	P	2.40	7/160 (4.4%)	4.05	17/243 (7.0%)
3	A	1.37	26/2672 (1.0%)	1.73	60/3590 (1.7%)
All	All	1.50	37/2994 (1.2%)	2.07	102/4082 (2.5%)

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	4	0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	DA	N9-C4	11.62	1.44	1.37
3	A	247	GLU	CD-OE1	10.36	1.37	1.25
1	T	1	DC	C3'-O3'	9.12	1.55	1.44
2	P	2	DC	C1'-N1	8.15	1.59	1.49
3	A	249	GLU	CD-OE2	7.81	1.34	1.25
3	A	203	GLU	CD-OE1	7.71	1.34	1.25
3	A	86	GLU	CD-OE1	7.36	1.33	1.25
3	A	316	GLU	CD-OE2	7.23	1.33	1.25
3	A	153	GLU	CD-OE2	7.16	1.33	1.25
3	A	216	GLU	CD-OE2	7.13	1.33	1.25
3	A	117	GLU	CD-OE2	7.09	1.33	1.25
3	A	26	GLU	CD-OE1	7.00	1.33	1.25
2	P	1	DT	P-O5'	6.93	1.66	1.59
3	A	335	GLU	CD-OE2	6.85	1.33	1.25
3	A	309	GLU	CD-OE2	6.70	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	147	GLU	CD-OE2	6.62	1.32	1.25
3	A	172	GLU	CD-OE2	6.60	1.32	1.25
3	A	295	GLU	CD-OE2	6.54	1.32	1.25
3	A	71	GLU	CD-OE1	6.54	1.32	1.25
3	A	288	GLU	CD-OE2	6.53	1.32	1.25
3	A	329	GLU	CD-OE2	6.53	1.32	1.25
3	A	186	GLU	CD-OE1	6.39	1.32	1.25
3	A	154	GLU	CD-OE2	6.38	1.32	1.25
3	A	58	GLU	CD-OE1	6.15	1.32	1.25
3	A	232	GLU	CD-OE2	6.05	1.32	1.25
1	T	5	DA	C5-C6	-5.99	1.35	1.41
2	P	3	DT	N1-C2	5.96	1.42	1.38
1	T	7	DA	N9-C4	-5.84	1.34	1.37
2	P	3	DT	N3-C4	-5.83	1.33	1.38
3	A	123	GLU	CD-OE1	5.33	1.31	1.25
2	P	3	DT	N1-C6	-5.23	1.34	1.38
3	A	9	GLU	CD-OE2	5.22	1.31	1.25
3	A	129	GLU	CD-OE1	5.18	1.31	1.25
3	A	326	LYS	CE-NZ	-5.16	1.36	1.49
1	T	5	DA	C3'-O3'	-5.16	1.37	1.44
2	P	3	DT	C1'-N1	5.16	1.55	1.49
3	A	75	GLU	CD-OE1	5.07	1.31	1.25

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	6	DT	C6-N1-C1'	-19.91	90.54	120.40
2	P	6	DT	C2-N1-C1'	19.43	149.28	118.20
2	P	1	DT	C6-N1-C1'	-18.99	91.91	120.40
2	P	2	DC	C2-N1-C1'	17.99	138.59	118.80
2	P	1	DT	C2-N1-C1'	17.63	146.41	118.20
1	T	4	DT	C6-N1-C1'	-16.75	95.28	120.40
2	P	2	DC	C6-N1-C1'	-15.51	102.18	120.80
1	T	4	DT	C2-N1-C1'	15.35	142.76	118.20
2	P	3	DT	C6-N1-C1'	-14.19	99.12	120.40
2	P	3	DT	C2-N1-C1'	14.08	140.72	118.20
2	P	7	DG	C8-N9-C1'	13.77	144.91	127.00
2	P	7	DG	C4-N9-C1'	-13.25	109.27	126.50
1	T	7	DA	C4-N9-C1'	-13.13	102.67	126.30
2	P	3	DT	P-O3'-C3'	12.13	134.26	119.70
1	T	7	DA	C8-N9-C1'	11.58	148.55	127.70
1	T	1	DC	P-O3'-C3'	10.11	131.83	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	5	DA	C8-N9-C1'	8.88	143.69	127.70
1	T	6	DG	O4'-C1'-N9	8.87	114.21	108.00
3	A	192	ASP	CB-CG-OD2	-8.80	110.38	118.30
2	P	3	DT	O4'-C1'-N1	8.62	114.03	108.00
3	A	142	TYR	CB-CG-CD1	-8.56	115.87	121.00
2	P	5	DA	C4-N9-C1'	8.26	141.17	126.30
1	T	5	DA	C4-N9-C1'	-8.19	111.56	126.30
2	P	2	DC	O4'-C1'-N1	8.13	113.69	108.00
1	T	2	DA	C8-N9-C1'	7.87	141.86	127.70
3	A	314	ASP	CB-CG-OD1	-7.65	111.41	118.30
1	T	2	DA	C4-N9-C1'	-7.62	112.59	126.30
3	A	263	ASP	CB-CG-OD2	-7.51	111.55	118.30
3	A	130	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	T	7	DA	C8-N9-C4	7.27	108.71	105.80
1	T	5	DA	N1-C6-N6	7.26	122.96	118.60
2	P	5	DA	C8-N9-C1'	-7.24	114.66	127.70
1	T	4	DT	C6-C5-C7	-7.21	118.58	122.90
3	A	190	ASP	CB-CG-OD2	-7.18	111.84	118.30
3	A	163	LEU	CA-CB-CG	-7.13	98.89	115.30
1	T	4	DT	O4'-C1'-N1	7.00	112.90	108.00
3	A	124	ASP	CB-CG-OD2	-6.98	112.01	118.30
1	T	2	DA	O4'-C1'-N9	6.97	112.88	108.00
3	A	92	ASP	N-CA-CB	6.88	122.98	110.60
3	A	332	ASP	CB-CG-OD1	-6.87	112.11	118.30
2	P	3	DT	N3-C2-O2	-6.80	118.22	122.30
3	A	92	ASP	CB-CG-OD2	-6.70	112.27	118.30
3	A	130	ASP	CB-CG-OD1	6.63	124.26	118.30
3	A	326	LYS	CD-CE-NZ	6.57	126.80	111.70
1	T	4	DT	C1'-O4'-C4'	-6.52	103.58	110.10
3	A	168	LYS	N-CA-CB	6.51	122.32	110.60
3	A	91	ASP	CB-CG-OD1	-6.49	112.46	118.30
3	A	222	HIS	CA-CB-CG	-6.48	102.58	113.60
3	A	27	LYS	CB-CA-C	6.38	123.15	110.40
1	T	1	DC	O4'-C1'-N1	6.36	112.45	108.00
1	T	6	DG	P-O3'-C3'	6.29	127.24	119.70
3	A	116	ASP	CB-CA-C	6.23	122.86	110.40
3	A	334	SER	N-CA-CB	6.20	119.80	110.50
3	A	22	LEU	CB-CG-CD1	-6.17	100.51	111.00
3	A	39	TYR	CB-CG-CD1	-6.17	117.30	121.00
3	A	92	ASP	CB-CG-OD1	6.16	123.84	118.30
3	A	314	ASP	CB-CG-OD2	6.13	123.81	118.30
3	A	116	ASP	CB-CG-OD1	6.08	123.77	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	190	ASP	CB-CG-OD1	6.03	123.72	118.30
3	A	74	ASP	CB-CG-OD2	-6.01	112.89	118.30
3	A	257	ILE	CB-CA-C	-5.96	99.68	111.60
3	A	333	ARG	NE-CZ-NH1	5.95	123.28	120.30
3	A	116	ASP	CB-CG-OD2	-5.94	112.96	118.30
3	A	157	GLN	N-CA-CB	5.85	121.13	110.60
3	A	74	ASP	CB-CG-OD1	5.84	123.55	118.30
3	A	102	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	T	6	DG	C4-N9-C1'	-5.83	118.93	126.50
3	A	91	ASP	N-CA-CB	5.73	120.91	110.60
3	A	224	ILE	CA-CB-CG1	-5.71	100.16	111.00
1	T	1	DC	O4'-C1'-C2'	5.69	110.45	105.90
3	A	271	TYR	CB-CG-CD1	-5.69	117.59	121.00
3	A	256	ASP	CB-CG-OD2	-5.64	113.22	118.30
3	A	196	THR	N-CA-CB	5.63	121.00	110.30
3	A	219	GLN	CB-CA-C	-5.60	99.19	110.40
3	A	314	ASP	N-CA-CB	5.60	120.69	110.60
3	A	299	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	A	276	ASP	CB-CG-OD1	5.56	123.30	118.30
3	A	253	ARG	NE-CZ-NH1	5.53	123.07	120.30
3	A	36	TYR	CA-CB-CG	-5.46	103.02	113.40
1	T	4	DT	C4-C5-C7	5.41	122.24	119.00
1	T	5	DA	C4-C5-N7	5.40	113.40	110.70
2	P	5	DA	C2-N3-C4	5.40	113.30	110.60
3	A	243	SER	CB-CA-C	5.38	120.33	110.10
3	A	266	TYR	CA-CB-CG	-5.38	103.18	113.40
3	A	332	ASP	CB-CG-OD2	5.35	123.11	118.30
3	A	17	ASP	CB-CA-C	5.34	121.09	110.40
3	A	315	SER	N-CA-CB	5.32	118.48	110.50
3	A	83	ARG	N-CA-CB	5.30	120.14	110.60
3	A	91	ASP	CB-CG-OD2	5.27	123.04	118.30
3	A	17	ASP	N-CA-CB	5.22	119.99	110.60
1	T	5	DA	C6-C5-N7	-5.20	128.66	132.30
1	T	4	DT	P-O5'-C5'	5.19	129.20	120.90
3	A	45	VAL	CA-CB-CG1	-5.17	103.14	110.90
3	A	276	ASP	CB-CG-OD2	-5.17	113.64	118.30
3	A	142	TYR	CB-CG-CD2	5.16	124.10	121.00
1	T	6	DG	C8-N9-C1'	5.14	133.68	127.00
3	A	258	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	A	170	ASP	CB-CG-OD1	5.12	122.91	118.30
3	A	145	ASP	CB-CG-OD2	-5.07	113.74	118.30
3	A	304	THR	CA-CB-CG2	-5.05	105.33	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	125	LEU	CA-CB-CG	-5.02	103.76	115.30
3	A	170	ASP	CB-CG-OD2	-5.01	113.80	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	17	ASP	CA
3	A	65	VAL	CA
3	A	92	ASP	CA
3	A	246	ASP	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	145	0	80	8	0
2	P	144	0	81	8	0
3	A	2623	0	2641	338	0
4	A	5	0	0	0	0
5	A	2	0	0	0	0
6	A	104	0	0	12	0
6	P	18	0	0	1	0
6	T	15	0	0	3	0
All	All	3056	0	2802	352	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 62.

All (352) 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:1:DT:H2''	2:P:2:DC:H5'	1.24	1.16
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.13	1.06
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.42	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:ASN:N	3:A:245:ASN:HD22	1.61	0.98
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.11	0.97
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.47	0.97
3:A:245:ASN:H	3:A:245:ASN:HD22	1.00	0.97
3:A:243:SER:HB3	3:A:249:GLU:HA	1.47	0.93
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.49	0.92
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.06	0.90
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.70	0.89
2:P:5:DA:H2''	2:P:6:DT:H5'	1.54	0.89
3:A:277:ILE:HD13	3:A:277:ILE:H	1.36	0.88
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.57	0.87
3:A:155:MET:HE2	3:A:188:SER:HB2	1.55	0.86
3:A:245:ASN:H	3:A:245:ASN:ND2	1.71	0.86
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.05	0.86
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.55	0.85
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.40	0.85
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.06	0.85
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.56	0.84
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.13	0.82
3:A:180:SER:HB3	3:A:183:ARG:NH2	1.94	0.81
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.62	0.81
3:A:11:LEU:HD23	3:A:11:LEU:H	1.45	0.80
3:A:243:SER:CB	3:A:249:GLU:HA	2.12	0.80
3:A:155:MET:HA	3:A:158:MET:CE	2.12	0.79
3:A:212:HIS:HB3	6:A:541:HOH:O	1.81	0.79
3:A:254:ARG:NH1	3:A:255:ILE:H	1.79	0.78
3:A:264:GLN:NE2	3:A:296:TYR:HB3	1.99	0.77
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.00	0.77
3:A:180:SER:CB	3:A:183:ARG:HH21	1.96	0.77
2:P:5:DA:H2''	2:P:6:DT:C5'	2.15	0.77
3:A:194:LEU:HD12	3:A:258:ARG:HG3	1.68	0.76
3:A:162:VAL:HG13	3:A:218:LEU:HD21	1.68	0.76
3:A:306:VAL:HG22	6:A:650:HOH:O	1.85	0.76
3:A:133:ASN:HD22	3:A:135:HIS:H	1.34	0.76
2:P:1:DT:C2'	2:P:2:DC:H5'	2.11	0.76
3:A:155:MET:HA	3:A:158:MET:HE3	1.67	0.75
3:A:180:SER:HA	3:A:183:ARG:HE	1.49	0.75
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.68	0.75
3:A:121:THR:HG23	3:A:124:ASP:CG	2.06	0.75
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.66	0.75
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.68	0.75
3:A:41:LYS:O	3:A:45:VAL:HG13	1.87	0.75
3:A:18:MET:O	3:A:21:GLU:HB2	1.87	0.74
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.69	0.74
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.52	0.74
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.17	0.74
3:A:41:LYS:HD3	3:A:42:ALA:N	2.03	0.74
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.18	0.73
6:P:568:HOH:O	3:A:110:ALA:HB2	1.89	0.73
3:A:133:ASN:ND2	3:A:135:HIS:H	1.86	0.73
3:A:323:ILE:O	3:A:324:GLN:HG2	1.89	0.72
3:A:155:MET:SD	3:A:158:MET:HE1	2.28	0.72
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.25	0.71
3:A:262:LYS:HG3	3:A:262:LYS:O	1.89	0.71
3:A:41:LYS:HD3	3:A:42:ALA:H	1.55	0.71
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.06	0.71
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.73	0.71
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.71	0.71
1:T:6:DG:H2"	1:T:7:DA:C8	2.26	0.71
3:A:12:ASN:HD21	3:A:53:ILE:H	1.37	0.70
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.73	0.70
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.22	0.70
3:A:270:LEU:HD21	3:A:282:MET:CE	2.21	0.70
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.27	0.70
3:A:12:ASN:HA	6:A:553:HOH:O	1.92	0.69
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.22	0.69
3:A:330:PRO:HA	3:A:333:ARG:CG	2.22	0.69
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.08	0.69
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.22	0.69
3:A:123:GLU:HG3	6:A:623:HOH:O	1.92	0.68
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.24	0.68
3:A:279:ASN:O	3:A:283:ARG:HG3	1.94	0.68
3:A:82:LEU:HB3	3:A:85:LEU:CB	2.24	0.68
3:A:294:ASN:O	3:A:296:TYR:N	2.27	0.68
3:A:166:VAL:HG13	3:A:173:TYR:HB3	1.76	0.67
3:A:122:LEU:O	3:A:126:ARG:HG3	1.94	0.66
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.87	0.66
3:A:79:THR:O	3:A:81:LYS:N	2.29	0.66
3:A:103:VAL:HA	6:A:600:HOH:O	1.95	0.65
3:A:121:THR:HG23	3:A:124:ASP:OD2	1.95	0.65
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.77	0.65
3:A:177:VAL:HG22	3:A:193:VAL:HG22	1.79	0.65
3:A:254:ARG:NH1	3:A:255:ILE:N	2.44	0.65
3:A:194:LEU:CD1	3:A:258:ARG:HG3	2.28	0.64
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.79	0.63
3:A:302:GLY:H	3:A:307:ALA:HB3	1.63	0.63
3:A:267:CYS:SG	3:A:297:THR:HA	2.38	0.63
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.81	0.63
3:A:41:LYS:NZ	3:A:64:GLY:O	2.29	0.63
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.80	0.63
3:A:327:TYR:HD1	3:A:328:ARG:N	1.97	0.63
3:A:121:THR:O	3:A:124:ASP:HB2	1.99	0.62
3:A:150:ILE:O	3:A:187:SER:HA	1.99	0.62
3:A:11:LEU:CD2	3:A:11:LEU:H	2.10	0.62
3:A:196:THR:OG1	3:A:197:HIS:N	2.32	0.62
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.32	0.62
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.30	0.62
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.81	0.62
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.29	0.62
1:T:3:DT:H1'	6:T:617:HOH:O	1.99	0.62
3:A:150:ILE:HD11	3:A:253:ARG:HG2	1.80	0.61
3:A:108:PRO:O	3:A:112:ARG:HG3	2.01	0.61
3:A:249:GLU:HG3	3:A:250:TYR:N	2.15	0.61
3:A:101:THR:HA	3:A:106:ILE:HG22	1.83	0.61
1:T:5:DA:H2''	1:T:6:DG:O5'	2.01	0.60
3:A:207:GLN:O	3:A:210:LEU:HB2	2.01	0.60
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.82	0.60
3:A:11:LEU:N	3:A:11:LEU:HD23	2.16	0.60
3:A:270:LEU:HD12	3:A:270:LEU:O	2.01	0.60
3:A:155:MET:CE	3:A:188:SER:HB2	2.29	0.59
3:A:164:ASN:O	3:A:168:LYS:HG2	2.03	0.59
3:A:123:GLU:O	3:A:127:LYS:HG2	2.02	0.59
3:A:306:VAL:HG23	3:A:307:ALA:N	2.17	0.59
3:A:174:ILE:O	3:A:195:LEU:HD12	2.02	0.59
3:A:25:PHE:CD2	3:A:88:ILE:HD13	2.38	0.59
3:A:278:PHE:HB2	3:A:333:ARG:O	2.03	0.59
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.33	0.59
3:A:73:ILE:CG2	3:A:77:LEU:HD22	2.28	0.59
3:A:149:ARG:NH2	3:A:188:SER:HA	2.18	0.59
3:A:326:LYS:O	3:A:326:LYS:HG3	2.02	0.59
3:A:217:GLN:O	3:A:220:LYS:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:CD2	3:A:319:ILE:HG21	2.33	0.58
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.33	0.58
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.33	0.58
3:A:165:GLU:O	3:A:168:LYS:N	2.37	0.58
3:A:315:SER:OG	3:A:316:GLU:N	2.36	0.58
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.04	0.57
3:A:248:LYS:HG2	3:A:248:LYS:O	2.05	0.57
3:A:277:ILE:HD13	3:A:277:ILE:N	2.15	0.57
3:A:292:THR:O	3:A:298:ILE:HA	2.03	0.57
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.70	0.57
3:A:265:TYR:O	3:A:268:GLY:N	2.38	0.57
3:A:295:GLU:OE1	3:A:295:GLU:N	2.36	0.57
3:A:35:LYS:O	3:A:38:ALA:HB3	2.04	0.57
3:A:18:MET:HE1	3:A:76:PHE:HB3	1.86	0.56
3:A:15:ILE:HG13	6:A:553:HOH:O	2.04	0.56
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.41	0.55
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.41	0.55
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.38	0.55
3:A:292:THR:O	3:A:298:ILE:HG13	2.07	0.55
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.27	0.55
1:T:4:DT:H1'	6:T:527:HOH:O	2.06	0.55
3:A:237:GLY:O	3:A:254:ARG:NH1	2.39	0.55
3:A:245:ASN:ND2	3:A:245:ASN:N	2.35	0.55
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.88	0.55
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.89	0.54
3:A:288:GLU:C	3:A:290:GLY:H	2.10	0.54
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.36	0.54
3:A:295:GLU:HA	6:A:592:HOH:O	2.07	0.54
3:A:122:LEU:C	3:A:122:LEU:HD23	2.27	0.54
3:A:286:ALA:O	3:A:291:PHE:N	2.41	0.54
1:T:2:DA:H2''	1:T:3:DT:OP2	2.08	0.54
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.87	0.54
3:A:299:ARG:CG	3:A:310:PRO:HD3	2.38	0.54
3:A:323:ILE:C	3:A:324:GLN:HG2	2.28	0.54
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.72	0.54
3:A:267:CYS:HG	3:A:297:THR:HA	1.72	0.54
3:A:302:GLY:N	3:A:307:ALA:HB3	2.22	0.54
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.89	0.54
3:A:218:LEU:CB	3:A:224:ILE:HD12	2.38	0.53
3:A:31:GLN:N	6:A:641:HOH:O	2.29	0.53
3:A:191:MET:HA	6:A:502:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:HIS:O	3:A:262:LYS:HB2	2.08	0.53
3:A:291:PHE:CE1	3:A:300:PRO:HA	2.43	0.53
3:A:286:ALA:O	3:A:291:PHE:HB2	2.08	0.53
3:A:286:ALA:HA	3:A:323:ILE:HG22	1.89	0.53
1:T:7:DA:N3	6:T:634:HOH:O	2.32	0.53
3:A:223:PHE:O	3:A:239:CYS:HA	2.09	0.53
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.23	0.53
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.90	0.53
3:A:21:GLU:OE1	3:A:85:LEU:HD21	2.09	0.53
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.44	0.53
3:A:59:ALA:O	3:A:62:LEU:HB2	2.08	0.53
3:A:124:ASP:O	3:A:128:ASN:ND2	2.28	0.53
3:A:41:LYS:O	3:A:44:SER:HB3	2.09	0.52
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.89	0.52
3:A:120:LYS:N	3:A:124:ASP:OD2	2.42	0.52
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.39	0.52
3:A:317:LYS:O	3:A:320:PHE:N	2.42	0.52
3:A:233:THR:HB	6:A:538:HOH:O	2.10	0.52
2:P:1:DT:H2''	2:P:2:DC:C5'	2.18	0.52
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.40	0.51
3:A:132:LEU:O	3:A:137:ARG:NE	2.44	0.51
3:A:114:PHE:HZ	3:A:132:LEU:HD23	1.75	0.51
3:A:218:LEU:HB3	3:A:224:ILE:HD12	1.93	0.51
3:A:331:LYS:HG2	3:A:332:ASP:N	2.19	0.51
3:A:45:VAL:HG21	3:A:63:PRO:O	2.10	0.51
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.16	0.51
3:A:114:PHE:CZ	3:A:132:LEU:HD23	2.46	0.51
3:A:27:LYS:HB2	3:A:36:TYR:CG	2.46	0.50
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.75	0.50
3:A:84:LYS:O	3:A:88:ILE:HG13	2.11	0.50
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.42	0.50
3:A:21:GLU:OE1	3:A:85:LEU:HD11	2.11	0.50
3:A:115:VAL:O	3:A:118:GLY:N	2.43	0.50
3:A:245:ASN:O	3:A:246:ASP:O	2.30	0.50
3:A:133:ASN:ND2	3:A:135:HIS:N	2.58	0.49
3:A:100:LEU:HD21	3:A:119:ILE:O	2.13	0.49
3:A:266:TYR:O	3:A:270:LEU:HB2	2.12	0.49
3:A:152:ARG:HA	3:A:155:MET:HB2	1.95	0.49
3:A:254:ARG:HH22	3:A:256:ASP:CG	2.14	0.49
3:A:270:LEU:HD23	3:A:319:ILE:HG21	1.94	0.49
3:A:152:ARG:NH2	3:A:181:PHE:O	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:ARG:HG2	3:A:310:PRO:HA	1.95	0.48
3:A:303:VAL:C	3:A:305:GLY:H	2.16	0.48
3:A:122:LEU:O	3:A:122:LEU:HD23	2.13	0.48
3:A:274:GLY:O	3:A:278:PHE:HD2	1.96	0.48
3:A:121:THR:HG23	3:A:124:ASP:OD1	2.13	0.48
3:A:127:LYS:HB2	3:A:128:ASN:HD21	1.78	0.48
3:A:18:MET:HE1	3:A:76:PHE:CB	2.43	0.48
3:A:309:GLU:N	3:A:309:GLU:OE1	2.46	0.48
3:A:150:ILE:N	3:A:188:SER:O	2.46	0.47
3:A:254:ARG:CZ	3:A:254:ARG:HB3	2.44	0.47
3:A:302:GLY:HA3	3:A:307:ALA:HB2	1.97	0.47
3:A:268:GLY:O	3:A:271:TYR:HB3	2.14	0.47
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.63	0.47
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.32	0.47
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.37	0.47
3:A:133:ASN:HD22	3:A:135:HIS:N	2.08	0.47
3:A:13:GLY:O	3:A:17:ASP:N	2.41	0.47
3:A:299:ARG:HG2	3:A:310:PRO:N	2.30	0.47
3:A:114:PHE:CZ	3:A:132:LEU:CD2	2.98	0.47
3:A:91:ASP:OD1	3:A:92:ASP:N	2.47	0.47
3:A:32:ALA:O	3:A:36:TYR:HB3	2.15	0.46
3:A:195:LEU:HB3	3:A:258:ARG:O	2.15	0.46
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.95	0.46
3:A:249:GLU:HG3	3:A:250:TYR:H	1.81	0.46
3:A:270:LEU:C	3:A:270:LEU:HD12	2.36	0.46
3:A:306:VAL:O	3:A:307:ALA:HB2	2.16	0.46
3:A:22:LEU:HD21	3:A:82:LEU:CD2	2.45	0.46
3:A:259:LEU:HD12	3:A:260:ILE:H	1.81	0.46
3:A:218:LEU:CD1	3:A:218:LEU:N	2.79	0.46
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.96	0.46
3:A:79:THR:C	3:A:81:LYS:H	2.17	0.46
3:A:211:LEU:O	3:A:211:LEU:HD12	2.15	0.46
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.97	0.46
3:A:26:GLU:HA	3:A:30:SER:OG	2.16	0.46
3:A:302:GLY:H	3:A:307:ALA:CB	2.29	0.46
3:A:282:MET:HE2	6:A:555:HOH:O	2.16	0.45
3:A:196:THR:HB	3:A:265:TYR:CD1	2.51	0.45
3:A:200:PHE:CE2	3:A:261:PRO:N	2.85	0.45
3:A:178:CYS:SG	3:A:194:LEU:HD22	2.57	0.45
3:A:22:LEU:HA	3:A:22:LEU:HD13	1.17	0.45
2:P:6:DT:H2'	2:P:6:DT:H6	0.91	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:163:LEU:HD23	3:A:163:LEU:N	2.19	0.45
3:A:77:LEU:HA	3:A:77:LEU:HD12	1.62	0.45
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.52	0.45
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.68	0.45
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.98	0.45
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.60	0.45
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.38	0.45
3:A:200:PHE:CE2	3:A:261:PRO:CA	3.00	0.45
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.31	0.45
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.46	0.45
3:A:136:GLN:H	3:A:136:GLN:HG3	1.49	0.45
3:A:15:ILE:O	3:A:19:LEU:HB2	2.17	0.45
3:A:212:HIS:CD2	3:A:212:HIS:N	2.83	0.45
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.32	0.45
3:A:223:PHE:CZ	3:A:239:CYS:SG	3.09	0.45
3:A:254:ARG:HH12	3:A:255:ILE:H	1.64	0.45
3:A:275:SER:OG	3:A:277:ILE:HD13	2.17	0.45
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.35	0.45
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.97	0.45
1:T:4:DT:O2	2:P:4:DA:H2	2.00	0.45
3:A:180:SER:HA	3:A:183:ARG:HB2	1.99	0.44
3:A:194:LEU:HD12	3:A:258:ARG:CG	2.43	0.44
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.17	0.44
3:A:298:ILE:HA	6:A:593:HOH:O	2.17	0.44
3:A:122:LEU:CD2	3:A:126:ARG:NH1	2.80	0.44
3:A:304:THR:HG23	3:A:304:THR:H	1.32	0.44
1:T:4:DT:N3	2:P:4:DA:C2	2.80	0.44
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.06	0.44
3:A:149:ARG:NH2	3:A:188:SER:CA	2.81	0.44
3:A:151:PRO:HG2	3:A:154:GLU:CD	2.38	0.44
3:A:154:GLU:OE2	3:A:250:TYR:HE1	2.00	0.44
3:A:119:ILE:HD13	3:A:119:ILE:HG23	1.74	0.44
3:A:138:ILE:HG22	3:A:138:ILE:O	2.18	0.44
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.52	0.44
3:A:260:ILE:HD12	3:A:260:ILE:HG23	1.57	0.44
3:A:216:GLU:O	3:A:220:LYS:HB2	2.17	0.44
3:A:253:ARG:NH1	3:A:253:ARG:CG	2.79	0.44
3:A:195:LEU:O	3:A:260:ILE:N	2.51	0.44
3:A:302:GLY:N	3:A:307:ALA:CB	2.80	0.44
3:A:317:LYS:HE3	3:A:321:ASP:OD1	2.17	0.44
3:A:19:LEU:HD23	3:A:43:ALA:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:33:ILE:H	3:A:33:ILE:HG22	1.41	0.43
3:A:82:LEU:HD23	3:A:85:LEU:HB2	2.01	0.43
3:A:119:ILE:CG2	3:A:124:ASP:CB	2.96	0.43
3:A:240:GLN:NE2	3:A:250:TYR:O	2.45	0.43
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.53	0.43
3:A:299:ARG:HG2	3:A:310:PRO:CA	2.48	0.43
3:A:83:ARG:O	3:A:86:GLU:N	2.52	0.43
3:A:165:GLU:HB3	3:A:217:GLN:HG2	1.99	0.43
3:A:198:PRO:C	3:A:200:PHE:H	2.21	0.43
3:A:68:LYS:O	3:A:72:LYS:HE3	2.19	0.43
3:A:27:LYS:CB	3:A:36:TYR:CD1	3.02	0.43
3:A:15:ILE:HB	3:A:46:ILE:HD13	1.97	0.43
3:A:165:GLU:HA	3:A:168:LYS:CG	2.44	0.43
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.44	0.43
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.32	0.43
3:A:165:GLU:OE2	3:A:168:LYS:HD3	2.18	0.42
3:A:286:ALA:HB2	3:A:293:ILE:HD11	2.01	0.42
3:A:122:LEU:HD22	3:A:126:ARG:NH1	2.34	0.42
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.65	0.42
3:A:258:ARG:H	3:A:258:ARG:HG2	1.47	0.42
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.35	0.42
3:A:191:MET:CG	3:A:255:ILE:HG13	2.32	0.42
3:A:29:VAL:HG21	3:A:94:SER:HB2	2.02	0.42
3:A:200:PHE:HE2	3:A:261:PRO:N	2.18	0.42
3:A:277:ILE:CG1	3:A:335:GLU:HB3	2.49	0.42
3:A:73:ILE:HG22	3:A:77:LEU:CD2	2.40	0.42
3:A:213:GLN:HB2	3:A:213:GLN:HE21	1.50	0.42
3:A:156:LEU:HD23	3:A:156:LEU:HA	1.88	0.42
3:A:163:LEU:HA	3:A:163:LEU:HD23	1.19	0.42
3:A:254:ARG:HH11	3:A:255:ILE:H	1.62	0.42
3:A:322:TYR:C	3:A:324:GLN:H	2.22	0.42
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.50	0.42
3:A:230:LYS:HA	3:A:235:PHE:HA	2.01	0.41
3:A:211:LEU:C	3:A:211:LEU:HD12	2.40	0.41
3:A:44:SER:O	3:A:47:ALA:HB3	2.19	0.41
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.36	0.41
3:A:151:PRO:HD2	3:A:154:GLU:OE1	2.21	0.41
3:A:182:ARG:NH1	3:A:182:ARG:HG2	2.36	0.41
3:A:18:MET:HG2	3:A:19:LEU:N	2.32	0.41
3:A:253:ARG:NH1	3:A:253:ARG:HG3	2.19	0.41
3:A:18:MET:HG2	3:A:22:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:243:SER:OG	3:A:249:GLU:HG3	2.21	0.41
3:A:212:HIS:CD2	3:A:212:HIS:H	2.39	0.41
3:A:217:GLN:HE22	3:A:220:LYS:HD3	1.85	0.41
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.68	0.41
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.23	0.41
3:A:62:LEU:HA	3:A:62:LEU:HD12	1.72	0.41
3:A:248:LYS:N	3:A:248:LYS:HD2	2.36	0.41
3:A:151:PRO:O	3:A:154:GLU:N	2.46	0.41
3:A:214:VAL:CG2	3:A:215:VAL:N	2.79	0.41
3:A:243:SER:OG	3:A:249:GLU:HA	2.21	0.41
3:A:200:PHE:CE2	3:A:261:PRO:HA	2.54	0.41
3:A:127:LYS:HG2	3:A:127:LYS:H	1.52	0.41
3:A:18:MET:CE	3:A:76:PHE:CB	2.99	0.41
3:A:327:TYR:CD1	3:A:328:ARG:N	2.84	0.41
3:A:34:HIS:O	3:A:37:ASN:N	2.54	0.41
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.44	0.40
3:A:40:ARG:HB2	3:A:40:ARG:HE	1.47	0.40
3:A:230:LYS:HB3	3:A:230:LYS:HE2	1.36	0.40
3:A:320:PHE:O	3:A:324:GLN:N	2.54	0.40
3:A:155:MET:CE	3:A:188:SER:CB	2.99	0.40
3:A:194:LEU:CD1	3:A:258:ARG:CG	2.99	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%)	258 (79%)	44 (14%)	23 (7%)	1 6

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	185	ALA
3	A	202	SER
3	A	204	SER
3	A	205	THR
3	A	244	LYS
3	A	246	ASP
3	A	265	TYR
3	A	266	TYR
3	A	295	GLU
3	A	247	GLU
3	A	10	THR
3	A	199	SER
3	A	206	LYS
3	A	289	LYS
3	A	316	GLU
3	A	80	GLY
3	A	207	GLN
3	A	91	ASP
3	A	222	HIS
3	A	310	PRO
3	A	166	VAL
3	A	309	GLU
3	A	50	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%)	218 (76%)	70 (24%)	0 2

All (70) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	27	LYS
3	A	33	ILE
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	77	LEU
3	A	79	THR
3	A	89	ARG
3	A	92	ASP
3	A	93	THR
3	A	94	SER
3	A	100	LEU
3	A	101	THR
3	A	104	SER
3	A	119	ILE
3	A	121	THR
3	A	126	ARG
3	A	133	ASN
3	A	152	ARG
3	A	153	GLU
3	A	155	MET
3	A	161	ILE
3	A	168	LYS
3	A	169	VAL
3	A	188	SER
3	A	191	MET
3	A	194	LEU
3	A	199	SER
3	A	201	THR
3	A	202	SER
3	A	205	THR
3	A	214	VAL
3	A	218	LEU
3	A	226	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	228	LEU
3	A	230	LYS
3	A	236	MET
3	A	242	PRO
3	A	245	ASN
3	A	248	LYS
3	A	249	GLU
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	262	LYS
3	A	264	GLN
3	A	277	ILE
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	301	LEU
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	327	TYR
3	A	331	LYS
3	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	133	ASN
3	A	135	HIS
3	A	136	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	222	HIS
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	294	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	338	-	4,4,4	1.16	0	6,6,6	0.83	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.96	0	100 100	25, 43, 99, 99	0
2	P	7/7 (100%)	-1.16	0	100 100	26, 34, 48, 81	0
3	A	326/335 (97%)	-1.22	1 (0%)	94 88	3, 36, 84, 100	0
All	All	341/350 (97%)	-1.22	1 (0%)	94 88	3, 36, 86, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	247	GLU	4.3

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. 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	SO4	A	338	5/5	0.96	0.22	41,44,48,49	5
5	NA	A	342	1/1	0.97	0.11	67,67,67,67	0
5	NA	A	341	1/1	0.99	0.06	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.