



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:39 AM GMT

PDB ID : 3PKP
Title : Q83S Variant of S. Enterica RmlA with dATP
Authors : Chang, A.; Moretti, R.; Bingman, C.A.; Thorson, J.S.; Phillips Jr., G.N.;
Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2010-11-11
Resolution : 2.60 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

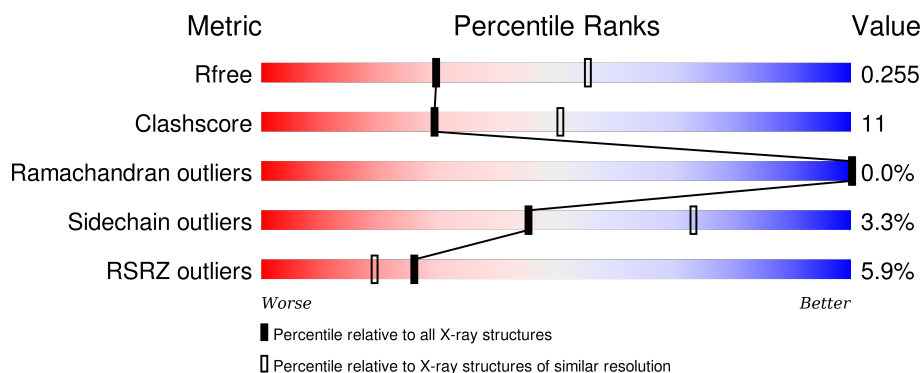
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	A	292	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	B	292	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>..</div> </div> </div>
1	C	292	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	D	292	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	I	292	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	292	<div><div></div><div>3%</div><div>73%</div><div>23%</div><div></div><div>• •</div></div>
1	K	292	<div><div></div><div>14%</div><div>75%</div><div>20%</div><div></div><div>• •</div></div>
1	L	292	<div><div></div><div>12%</div><div>74%</div><div>22%</div><div></div><div>• •</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18344 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

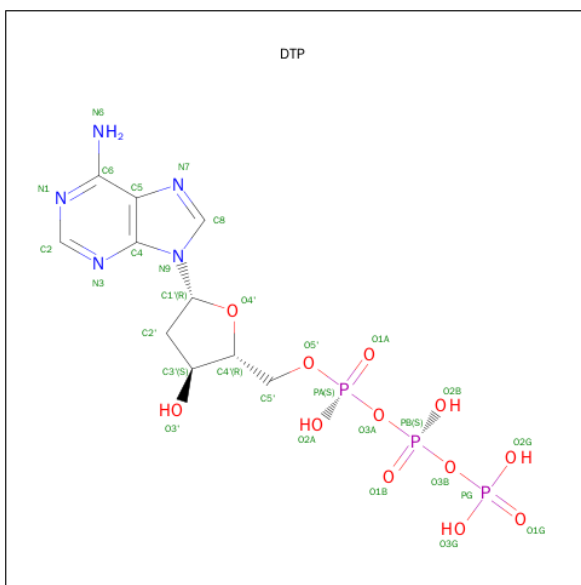
- Molecule 1 is a protein called Glucose-1-phosphate thymidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2267	1451	377	427	12			
1	B	289	Total	C	N	O	S	0	0	0
			2259	1446	376	426	11			
1	C	282	Total	C	N	O	S	0	0	0
			2208	1415	364	418	11			
1	D	283	Total	C	N	O	S	0	0	0
			2217	1421	366	419	11			
1	I	289	Total	C	N	O	S	0	0	0
			2259	1446	376	426	11			
1	J	289	Total	C	N	O	S	0	0	0
			2259	1446	376	426	11			
1	K	284	Total	C	N	O	S	0	0	0
			2223	1426	369	417	11			
1	L	284	Total	C	N	O	S	0	0	0
			2226	1427	368	420	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	SER	GLN	ENGINEERED MUTATION	UNP P26393
B	83	SER	GLN	ENGINEERED MUTATION	UNP P26393
C	83	SER	GLN	ENGINEERED MUTATION	UNP P26393
D	83	SER	GLN	ENGINEERED MUTATION	UNP P26393
I	83	SER	GLN	ENGINEERED MUTATION	UNP P26393
J	83	SER	GLN	variant	UNP P26393
K	83	SER	GLN	variant	UNP P26393
L	83	SER	GLN	variant	UNP P26393

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	D	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	I	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	J	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	K	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	L	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	K	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0
3	L	2	Total 2	Mg 2	0	0

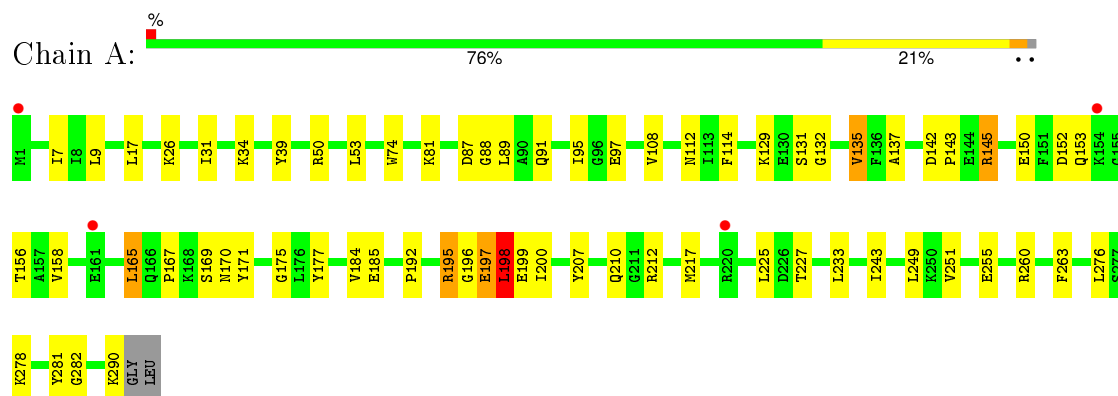
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total 45	O 45	0	0
4	B	31	Total 31	O 31	0	0
4	C	11	Total 11	O 11	0	0
4	D	10	Total 10	O 10	0	0
4	I	35	Total 35	O 35	0	0
4	J	30	Total 30	O 30	0	0
4	K	4	Total 4	O 4	0	0
4	L	4	Total 4	O 4	0	0

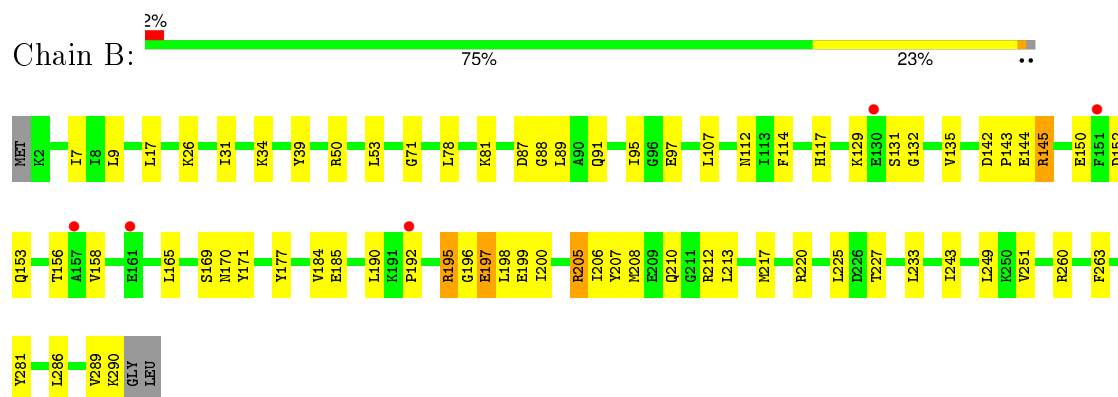
3 Residue-property plots

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

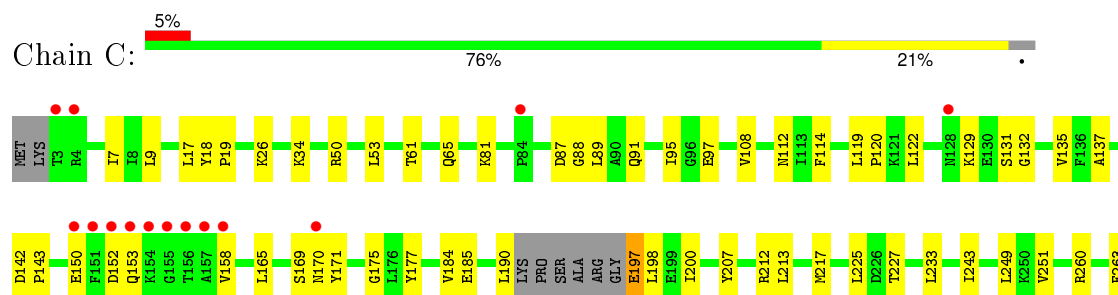
- Molecule 1: Glucose-1-phosphate thymidyltransferase

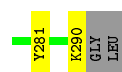


- Molecule 1: Glucose-1-phosphate thymidyltransferase

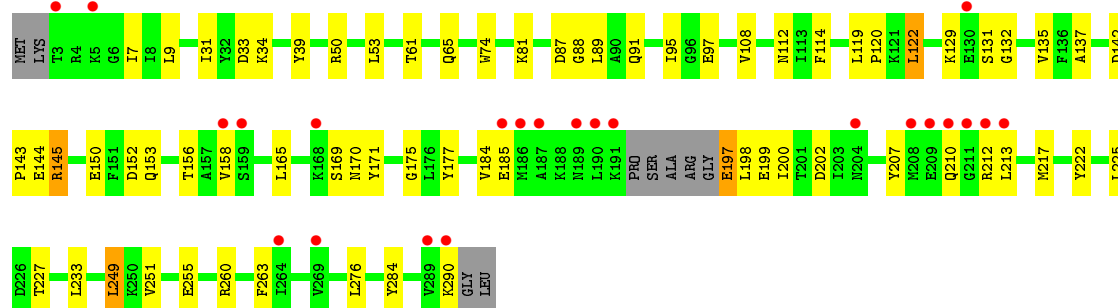
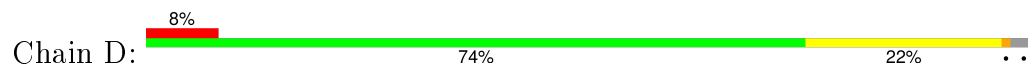


- Molecule 1: Glucose-1-phosphate thymidyltransferase

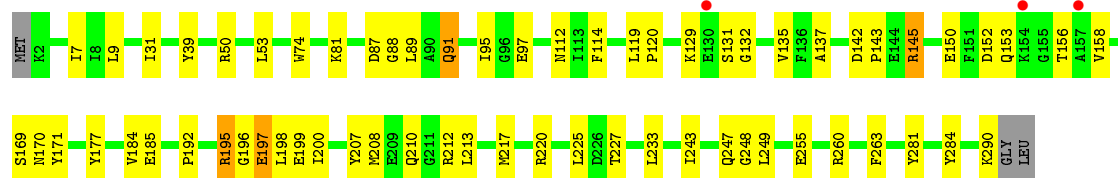
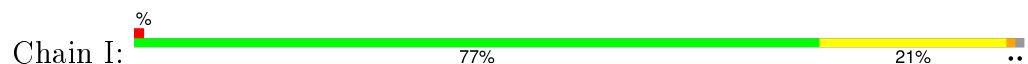




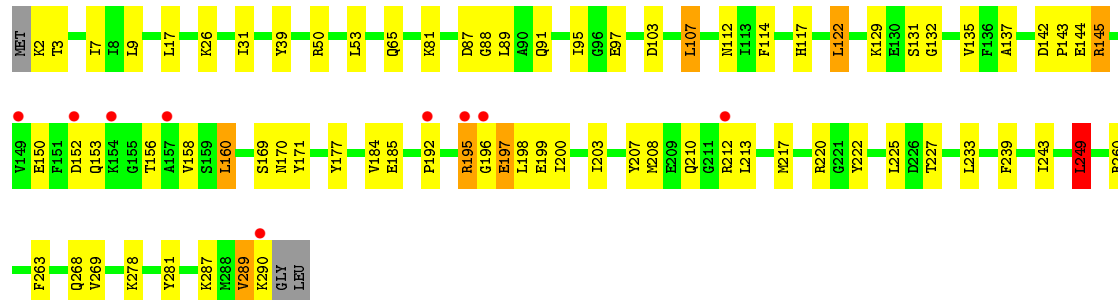
• Molecule 1: Glucose-1-phosphate thymidyltransferase



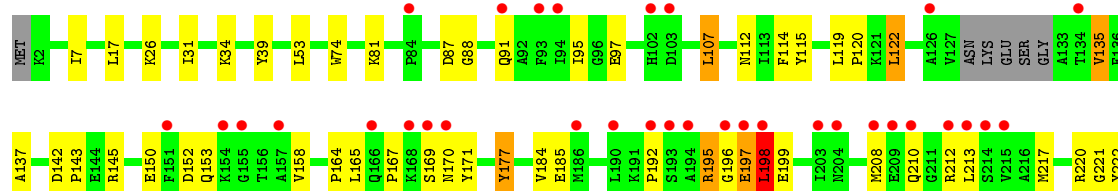
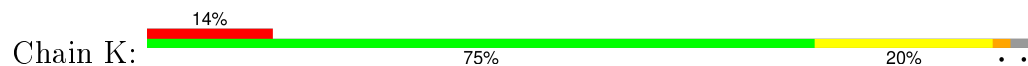
• Molecule 1: Glucose-1-phosphate thymidyltransferase

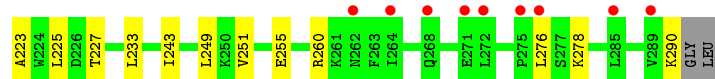


• Molecule 1: Glucose-1-phosphate thymidyltransferase

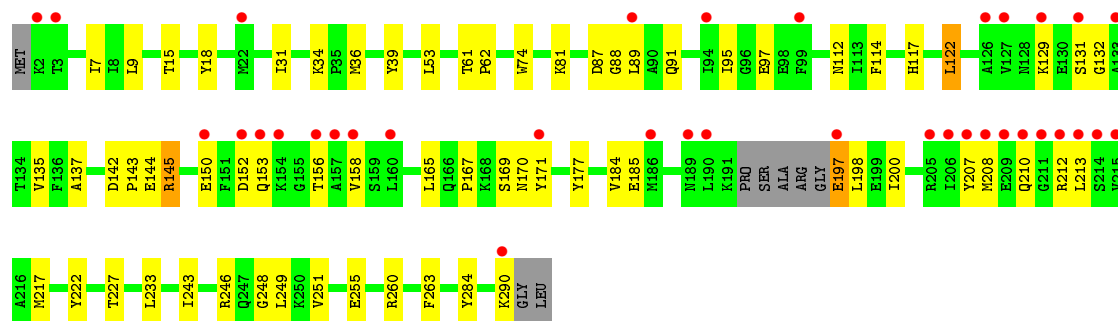
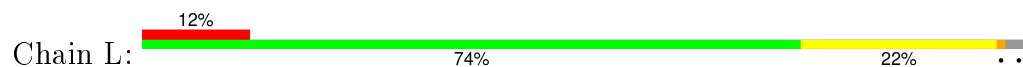


• Molecule 1: Glucose-1-phosphate thymidyltransferase





- Molecule 1: Glucose-1-phosphate thymidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.88Å 134.31Å 175.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.39 – 2.60 43.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.4 (43.39-2.60) 89.7 (43.39-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.200 , 0.260 0.202 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (2.84%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77487 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18344	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/2314	0.64	2/3131 (0.1%)
1	B	0.46	0/2306	0.63	1/3121 (0.0%)
1	C	0.39	0/2253	0.60	1/3050 (0.0%)
1	D	0.39	0/2262	0.58	0/3061
1	I	0.45	0/2306	0.61	0/3121
1	J	0.45	0/2306	0.64	3/3121 (0.1%)
1	K	0.43	0/2269	0.65	4/3071 (0.1%)
1	L	0.40	0/2271	0.58	0/3072
All	All	0.43	0/18287	0.62	11/24748 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	LEU	CA-CB-CG	5.84	128.74	115.30
1	K	198	LEU	CB-CG-CD2	5.78	120.83	111.00
1	A	135	VAL	CG1-CB-CG2	5.78	120.15	110.90
1	K	135	VAL	CG1-CB-CG2	5.76	120.11	110.90
1	K	225	LEU	CA-CB-CG	5.72	128.47	115.30
1	A	198	LEU	CB-CG-CD2	5.28	119.97	111.00
1	C	225	LEU	CA-CB-CG	5.25	127.36	115.30
1	J	107	LEU	CB-CG-CD2	5.24	119.90	111.00
1	J	249	LEU	CB-CG-CD2	5.24	119.90	111.00
1	K	107	LEU	CB-CG-CD2	5.18	119.80	111.00
1	J	160	LEU	CB-CG-CD1	5.11	119.68	111.00

There are no chirality outliers.

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	A	2267	0	2279	50	0
1	B	2259	0	2267	59	0
1	C	2208	0	2207	44	0
1	D	2217	0	2220	46	0
1	I	2259	0	2267	52	0
1	J	2259	0	2267	69	0
1	K	2223	0	2233	54	0
1	L	2226	0	2233	55	0
2	A	30	0	12	0	0
2	B	30	0	12	0	0
2	C	30	0	12	1	0
2	D	30	0	12	0	0
2	I	30	0	12	0	0
2	J	30	0	12	1	0
2	K	30	0	12	1	0
2	L	30	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	45	0	0	3	0
4	B	31	0	0	1	0
4	C	11	0	0	0	0
4	D	10	0	0	0	0
4	I	35	0	0	1	0
4	J	30	0	0	2	0
4	K	4	0	0	0	0
4	L	4	0	0	2	0
All	All	18344	0	18069	409	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 11.

All (409) 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)
1:B:205:ARG:HG3	1:B:208:MET:CE	1.50	1.39
1:J:2:LYS:O	1:J:3:THR:HG23	1.39	1.23
1:B:205:ARG:CG	1:B:208:MET:HE2	1.83	1.09
1:B:205:ARG:CG	1:B:208:MET:CE	2.32	1.05
1:J:287:LYS:O	1:J:290:LYS:HG2	1.58	1.02
1:J:2:LYS:O	1:J:3:THR:CG2	2.22	0.85
1:B:205:ARG:HG3	1:B:208:MET:HE2	0.87	0.85
1:L:117:HIS:CD2	4:L:296:HOH:O	2.30	0.83
1:D:260:ARG:HG3	1:D:260:ARG:HH11	1.43	0.82
1:I:260:ARG:HG3	1:I:260:ARG:HH11	1.44	0.82
1:K:260:ARG:HH11	1:K:260:ARG:HG3	1.44	0.81
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.47	0.80
1:B:260:ARG:HG3	1:B:260:ARG:HH11	1.43	0.80
1:C:260:ARG:HH11	1:C:260:ARG:HG3	1.47	0.80
1:L:129:LYS:HE2	1:L:131:SER:O	1.82	0.80
1:J:260:ARG:HH11	1:J:260:ARG:HG3	1.45	0.80
1:B:129:LYS:HE2	1:B:131:SER:O	1.83	0.79
1:C:129:LYS:HE2	1:C:131:SER:O	1.82	0.78
1:J:287:LYS:O	1:J:290:LYS:CG	2.31	0.78
1:I:129:LYS:HE2	1:I:131:SER:O	1.84	0.78
1:J:129:LYS:HE2	1:J:131:SER:O	1.84	0.78
1:D:129:LYS:HE2	1:D:131:SER:O	1.83	0.77
1:A:129:LYS:HE2	1:A:131:SER:O	1.84	0.77
1:D:198:LEU:HD12	1:D:198:LEU:H	1.51	0.76
1:L:260:ARG:HH11	1:L:260:ARG:HG3	1.50	0.76
1:D:198:LEU:N	1:D:198:LEU:HD12	2.01	0.76
1:B:286:LEU:O	1:B:289:VAL:HG22	1.88	0.73
1:L:198:LEU:HD12	1:L:198:LEU:N	2.05	0.71
1:K:88:GLY:O	1:K:91:GLN:HB2	1.91	0.70
1:L:88:GLY:O	1:L:91:GLN:HB2	1.90	0.70
1:B:143:PRO:HG3	1:B:170:ASN:HA	1.72	0.70
1:K:97:GLU:HG3	1:K:184:VAL:HG11	1.75	0.69
1:B:249:LEU:O	1:B:249:LEU:HD12	1.91	0.69
1:B:198:LEU:N	1:B:198:LEU:HD12	2.06	0.69
1:A:143:PRO:HG3	1:A:170:ASN:HA	1.75	0.69
1:I:143:PRO:HG3	1:I:170:ASN:HA	1.74	0.68
1:C:198:LEU:HD12	1:C:198:LEU:N	2.08	0.68
1:D:81:LYS:HG2	1:D:95:ILE:CG2	2.24	0.67
1:A:249:LEU:O	1:A:249:LEU:HD12	1.92	0.67
1:C:88:GLY:O	1:C:91:GLN:HB2	1.94	0.67
1:J:143:PRO:HG3	1:J:170:ASN:HA	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:198:LEU:HD12	1:J:198:LEU:N	2.08	0.67
1:C:143:PRO:HG3	1:C:170:ASN:HA	1.77	0.67
1:D:88:GLY:O	1:D:91:GLN:HB2	1.95	0.66
1:K:143:PRO:HG3	1:K:170:ASN:HA	1.77	0.66
1:I:284:TYR:CZ	1:K:220:ARG:NH1	2.64	0.66
1:J:97:GLU:HG3	1:J:184:VAL:HG11	1.78	0.66
1:D:260:ARG:HG3	1:D:260:ARG:NH1	2.11	0.65
1:I:88:GLY:O	1:I:91:GLN:HB2	1.95	0.65
2:J:500:DTP:O2G	2:J:500:DTP:O2B	2.13	0.65
1:K:192:PRO:HB3	1:K:196:GLY:C	2.18	0.65
1:A:88:GLY:O	1:A:91:GLN:HB2	1.95	0.64
1:J:220:ARG:HB2	1:L:248:GLY:O	1.98	0.64
1:B:205:ARG:CG	1:B:208:MET:HE3	2.25	0.64
1:L:143:PRO:HG3	1:L:170:ASN:HA	1.79	0.64
1:D:97:GLU:HG3	1:D:184:VAL:HG11	1.79	0.64
1:J:88:GLY:O	1:J:91:GLN:HB2	1.97	0.64
1:J:260:ARG:NH1	1:J:260:ARG:HG3	2.13	0.64
1:K:81:LYS:HG2	1:K:95:ILE:CG2	2.28	0.64
1:J:287:LYS:HA	1:J:290:LYS:HD3	1.80	0.63
1:B:88:GLY:O	1:B:91:GLN:HB2	1.98	0.63
1:K:249:LEU:HD12	1:K:249:LEU:O	1.98	0.63
1:I:152:ASP:OD1	1:I:153:GLN:N	2.31	0.63
1:C:81:LYS:HG2	1:C:95:ILE:CG2	2.27	0.63
2:C:500:DTP:O2G	2:C:500:DTP:O2B	2.14	0.63
1:C:260:ARG:NH1	1:C:260:ARG:HG3	2.14	0.63
1:I:89:LEU:HB3	1:I:200:ILE:HD11	1.80	0.63
1:B:152:ASP:OD1	1:B:153:GLN:N	2.32	0.63
1:B:205:ARG:HG3	1:B:208:MET:HE3	1.68	0.62
1:L:81:LYS:HG2	1:L:95:ILE:CG2	2.30	0.62
1:L:97:GLU:HG3	1:L:184:VAL:HG11	1.80	0.62
1:C:97:GLU:HG3	1:C:184:VAL:HG11	1.81	0.62
1:D:198:LEU:H	1:D:198:LEU:CD1	2.12	0.62
1:C:152:ASP:OD1	1:C:153:GLN:N	2.33	0.62
1:J:117:HIS:CD2	4:L:296:HOH:O	2.52	0.62
1:K:260:ARG:HG3	1:K:260:ARG:NH1	2.13	0.62
1:B:192:PRO:HB3	1:B:196:GLY:C	2.20	0.62
1:I:198:LEU:HD12	1:I:198:LEU:N	2.14	0.62
1:D:143:PRO:HG3	1:D:170:ASN:HA	1.81	0.62
1:J:287:LYS:C	1:J:290:LYS:HG2	2.20	0.61
1:L:152:ASP:OD1	1:L:153:GLN:N	2.33	0.61
1:J:287:LYS:HA	1:J:290:LYS:CD	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:O	1:C:249:LEU:HD12	1.99	0.61
1:J:89:LEU:HB3	1:J:200:ILE:HD11	1.81	0.61
1:B:97:GLU:HG3	1:B:184:VAL:HG11	1.81	0.61
1:D:152:ASP:OD1	1:D:153:GLN:N	2.33	0.61
1:J:152:ASP:OD1	1:J:153:GLN:N	2.34	0.61
1:A:89:LEU:HB3	1:A:200:ILE:HD11	1.81	0.61
1:I:249:LEU:O	1:I:249:LEU:HD12	2.01	0.61
1:I:81:LYS:HG2	1:I:95:ILE:CG2	2.31	0.61
1:A:260:ARG:HG3	1:A:260:ARG:NH1	2.15	0.61
1:A:198:LEU:H	1:A:198:LEU:HD23	1.66	0.61
1:J:81:LYS:HG2	1:J:95:ILE:CG2	2.31	0.61
1:A:197:GLU:HB3	4:A:322:HOH:O	1.99	0.61
1:L:260:ARG:HG3	1:L:260:ARG:NH1	2.16	0.60
1:I:243:ILE:CD1	1:K:243:ILE:HD11	2.31	0.60
1:J:192:PRO:HB3	1:J:196:GLY:C	2.22	0.60
1:L:89:LEU:HB3	1:L:200:ILE:HD11	1.84	0.60
1:I:97:GLU:HG3	1:I:184:VAL:HG11	1.83	0.60
1:L:198:LEU:HD12	1:L:198:LEU:H	1.65	0.60
1:C:198:LEU:HD12	1:C:198:LEU:H	1.67	0.60
1:C:18:TYR:HB3	1:D:276:LEU:CD2	2.32	0.60
1:A:152:ASP:OD1	1:A:153:GLN:N	2.34	0.59
1:I:192:PRO:HB3	1:I:196:GLY:C	2.22	0.59
1:K:152:ASP:OD1	1:K:153:GLN:N	2.36	0.59
1:B:260:ARG:HG3	1:B:260:ARG:NH1	2.11	0.59
1:K:198:LEU:H	1:K:198:LEU:HD23	1.68	0.59
1:B:198:LEU:HD12	1:B:198:LEU:H	1.66	0.58
1:C:18:TYR:HB3	1:D:276:LEU:HD23	1.85	0.58
1:B:81:LYS:HG2	1:B:95:ILE:CG2	2.33	0.58
1:C:89:LEU:HB3	1:C:200:ILE:HD11	1.85	0.58
1:I:260:ARG:HG3	1:I:260:ARG:NH1	2.11	0.58
1:A:81:LYS:HG2	1:A:95:ILE:CG2	2.33	0.58
1:A:97:GLU:HG3	1:A:184:VAL:HG11	1.84	0.58
1:A:192:PRO:HB3	1:A:196:GLY:C	2.23	0.58
1:C:34:LYS:HE2	1:C:251:VAL:O	2.03	0.58
1:J:243:ILE:HD11	1:L:243:ILE:CD1	2.34	0.58
1:K:122:LEU:HD22	1:K:222:TYR:OH	2.04	0.57
1:J:198:LEU:H	1:J:198:LEU:HD12	1.69	0.57
1:I:249:LEU:HD23	1:K:221:GLY:HA2	1.87	0.57
1:J:2:LYS:N	1:J:103:ASP:OD1	2.38	0.57
1:B:249:LEU:HD12	1:B:249:LEU:C	2.25	0.56
1:K:34:LYS:HE2	1:K:251:VAL:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:243:ILE:HD11	1:K:243:ILE:CD1	2.35	0.55
1:A:198:LEU:CD2	1:A:198:LEU:N	2.70	0.55
1:I:185:GLU:HA	1:I:185:GLU:OE1	2.07	0.55
1:D:185:GLU:HA	1:D:185:GLU:OE1	2.06	0.54
1:I:284:TYR:OH	1:K:220:ARG:NH1	2.40	0.54
1:B:205:ARG:O	1:B:206:ILE:C	2.42	0.54
1:J:243:ILE:CD1	1:L:243:ILE:HD11	2.38	0.54
1:J:268:GLN:HB3	4:J:303:HOH:O	2.07	0.53
1:A:185:GLU:OE1	1:A:185:GLU:HA	2.07	0.53
1:A:249:LEU:C	1:A:249:LEU:HD12	2.29	0.53
1:K:198:LEU:CD2	1:K:198:LEU:N	2.71	0.53
1:L:185:GLU:OE1	1:L:185:GLU:HA	2.09	0.53
1:L:198:LEU:H	1:L:198:LEU:CD1	2.22	0.53
1:B:143:PRO:CG	1:B:170:ASN:HA	2.39	0.52
1:B:243:ILE:HG22	1:B:249:LEU:HD11	1.92	0.52
1:C:50:ARG:HD3	1:C:263:PHE:CE1	2.45	0.52
1:B:185:GLU:OE1	1:B:185:GLU:HA	2.10	0.52
1:I:243:ILE:HD11	1:K:243:ILE:HD11	1.92	0.52
1:D:34:LYS:HE2	1:D:251:VAL:O	2.10	0.52
1:I:243:ILE:HG22	1:I:249:LEU:HD11	1.92	0.52
1:K:185:GLU:OE1	1:K:185:GLU:HA	2.09	0.52
1:J:210:GLN:OE1	1:J:212:ARG:NH1	2.43	0.51
1:K:227:THR:CG2	1:K:233:LEU:HD13	2.40	0.51
1:J:132:GLY:HA2	1:J:207:TYR:CE2	2.45	0.51
1:C:185:GLU:HA	1:C:185:GLU:OE1	2.09	0.51
1:K:249:LEU:HD12	1:K:249:LEU:C	2.31	0.51
1:K:276:LEU:HD23	1:L:18:TYR:HB3	1.91	0.51
1:A:50:ARG:HD3	1:A:263:PHE:CE1	2.45	0.51
1:K:243:ILE:HG22	1:K:249:LEU:HD11	1.93	0.51
1:D:50:ARG:HD3	1:D:263:PHE:CE1	2.46	0.51
1:C:249:LEU:C	1:C:249:LEU:HD12	2.32	0.51
1:K:195:ARG:NH2	1:K:199:GLU:OE2	2.44	0.51
1:L:132:GLY:HA2	1:L:207:TYR:CE2	2.46	0.51
1:L:198:LEU:CD1	1:L:198:LEU:N	2.71	0.51
1:J:185:GLU:HA	1:J:185:GLU:OE1	2.10	0.51
1:J:278:LYS:NZ	4:J:313:HOH:O	2.41	0.50
1:K:171:TYR:CE1	1:K:217:MET:HG3	2.47	0.50
1:A:243:ILE:HG22	1:A:249:LEU:HD11	1.93	0.50
1:K:143:PRO:CG	1:K:170:ASN:HA	2.40	0.50
1:I:248:GLY:O	1:K:220:ARG:HB2	2.11	0.50
1:A:198:LEU:HD23	4:A:297:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:ARG:O	1:J:197:GLU:HG2	2.12	0.50
1:J:122:LEU:HD22	1:J:222:TYR:OH	2.12	0.49
1:J:195:ARG:NH2	1:J:199:GLU:OE2	2.44	0.49
1:K:208:MET:HB2	1:K:213:LEU:HD23	1.94	0.49
1:D:227:THR:CG2	1:D:233:LEU:HD13	2.42	0.49
1:D:171:TYR:CE1	1:D:217:MET:HG3	2.47	0.49
1:K:227:THR:HG23	1:K:233:LEU:HA	1.94	0.49
1:J:112:ASN:HB3	1:J:114:PHE:CE1	2.47	0.49
1:D:7:ILE:HG12	1:D:53:LEU:HB3	1.94	0.49
1:I:249:LEU:C	1:I:249:LEU:HD12	2.33	0.49
1:B:198:LEU:CD1	1:B:198:LEU:H	2.25	0.49
1:A:143:PRO:CG	1:A:170:ASN:HA	2.40	0.49
1:K:87:ASP:HB3	1:K:197:GLU:OE1	2.13	0.49
1:L:9:LEU:HD13	1:L:89:LEU:HG	1.95	0.49
1:D:199:GLU:HB2	1:D:202:ASP:OD2	2.13	0.49
1:J:2:LYS:C	1:J:3:THR:HG23	2.24	0.48
1:C:198:LEU:H	1:C:198:LEU:CD1	2.26	0.48
1:I:198:LEU:H	1:I:198:LEU:HD12	1.78	0.48
1:D:132:GLY:HA2	1:D:207:TYR:CE2	2.48	0.48
1:B:117:HIS:CD2	4:B:319:HOH:O	2.66	0.48
1:A:227:THR:HG23	1:A:233:LEU:HA	1.95	0.48
1:A:278:LYS:NZ	4:A:331:HOH:O	2.39	0.48
1:C:132:GLY:HA2	1:C:207:TYR:CE2	2.48	0.48
1:I:132:GLY:HA2	1:I:207:TYR:CE2	2.48	0.48
1:J:198:LEU:CD1	1:J:198:LEU:N	2.75	0.48
1:K:198:LEU:CD2	1:K:198:LEU:H	2.27	0.48
1:K:7:ILE:HG12	1:K:53:LEU:HB3	1.96	0.48
1:K:115:TYR:HB3	1:K:223:ALA:HB3	1.96	0.48
1:J:198:LEU:H	1:J:198:LEU:CD1	2.26	0.48
1:B:208:MET:HB2	1:B:213:LEU:HD23	1.95	0.48
1:J:243:ILE:CD1	1:L:243:ILE:CD1	2.91	0.48
1:J:17:LEU:HD12	1:J:26:LYS:HD3	1.96	0.48
1:C:135:VAL:HG13	1:C:213:LEU:HD11	1.96	0.48
1:L:227:THR:HG23	1:L:233:LEU:HA	1.95	0.48
1:C:143:PRO:CG	1:C:170:ASN:HA	2.44	0.48
1:C:227:THR:HG23	1:C:233:LEU:HA	1.95	0.48
1:B:132:GLY:HA2	1:B:207:TYR:CE2	2.49	0.48
1:I:143:PRO:CG	1:I:170:ASN:HA	2.41	0.48
1:C:198:LEU:CD1	1:C:198:LEU:N	2.75	0.48
1:A:198:LEU:H	1:A:198:LEU:CD2	2.26	0.48
1:L:243:ILE:HG22	1:L:249:LEU:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:249:LEU:O	1:L:249:LEU:HD12	2.14	0.47
1:D:144:GLU:HG2	1:D:145:ARG:HG2	1.96	0.47
1:B:135:VAL:HG13	1:B:213:LEU:HD11	1.96	0.47
1:A:34:LYS:HE2	1:A:251:VAL:O	2.15	0.47
1:D:135:VAL:HG13	1:D:213:LEU:HD11	1.95	0.47
1:J:142:ASP:OD1	1:J:142:ASP:N	2.47	0.47
1:I:171:TYR:CE1	1:I:217:MET:HG3	2.49	0.47
1:I:135:VAL:HG13	1:I:213:LEU:HD11	1.97	0.47
1:I:195:ARG:NH2	1:I:199:GLU:OE2	2.47	0.47
1:I:227:THR:CG2	1:I:233:LEU:HD13	2.45	0.47
1:I:50:ARG:HD3	1:I:263:PHE:CE1	2.49	0.47
1:A:195:ARG:NH2	1:A:199:GLU:OE2	2.47	0.47
1:D:227:THR:HG23	1:D:233:LEU:HA	1.96	0.47
1:B:17:LEU:HD12	1:B:26:LYS:HD3	1.97	0.47
1:A:177:TYR:N	1:A:177:TYR:CD1	2.83	0.47
1:D:9:LEU:HD13	1:D:89:LEU:HD13	1.96	0.47
1:B:192:PRO:HB3	1:B:197:GLU:N	2.30	0.47
1:A:87:ASP:HB3	1:A:197:GLU:OE1	2.15	0.47
1:A:243:ILE:HD11	1:C:243:ILE:CD1	2.45	0.46
1:J:171:TYR:CE1	1:J:217:MET:HG3	2.50	0.46
1:B:195:ARG:NH2	1:B:199:GLU:OE2	2.49	0.46
1:L:87:ASP:HB3	1:L:197:GLU:OE1	2.15	0.46
1:A:210:GLN:OE1	1:A:212:ARG:NH1	2.48	0.46
1:B:87:ASP:HB3	1:B:197:GLU:OE1	2.16	0.46
1:L:135:VAL:HG13	1:L:213:LEU:HD11	1.97	0.46
1:D:31:ILE:HB	1:D:39:TYR:CE1	2.51	0.46
1:A:171:TYR:CE1	1:A:217:MET:HG3	2.50	0.46
1:A:112:ASN:HB3	1:A:114:PHE:CE1	2.51	0.46
1:C:87:ASP:HB3	1:C:197:GLU:OE1	2.14	0.46
1:D:122:LEU:HD22	1:D:222:TYR:OH	2.16	0.46
1:L:7:ILE:HG12	1:L:53:LEU:HB3	1.98	0.46
1:L:150:GLU:O	1:L:158:VAL:HG22	2.16	0.46
1:I:220:ARG:NH2	4:I:317:HOH:O	2.47	0.46
1:I:74:TRP:NE1	1:I:255:GLU:HG3	2.31	0.46
1:J:135:VAL:HG13	1:J:213:LEU:HD11	1.98	0.46
1:K:17:LEU:HD12	1:K:26:LYS:HD3	1.96	0.46
1:A:142:ASP:N	1:A:142:ASP:OD1	2.49	0.46
1:C:243:ILE:HG22	1:C:249:LEU:HD11	1.98	0.46
1:C:177:TYR:N	1:C:177:TYR:CD1	2.84	0.46
1:D:87:ASP:HB3	1:D:197:GLU:OE1	2.15	0.46
1:I:210:GLN:OE1	1:I:212:ARG:NH1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:HB2	1:A:145:ARG:HG3	1.98	0.46
1:C:150:GLU:O	1:C:158:VAL:HG22	2.16	0.46
1:I:150:GLU:O	1:I:158:VAL:HG22	2.16	0.45
1:D:177:TYR:CD1	1:D:177:TYR:N	2.84	0.45
1:L:31:ILE:HD11	1:L:36:MET:HE2	1.98	0.45
1:L:34:LYS:HE2	1:L:251:VAL:O	2.15	0.45
1:D:50:ARG:HD3	1:D:263:PHE:CZ	2.51	0.45
1:J:50:ARG:HD3	1:J:263:PHE:CE1	2.51	0.45
1:J:143:PRO:CG	1:J:170:ASN:HA	2.45	0.45
1:I:9:LEU:HD13	1:I:89:LEU:HG	1.99	0.45
1:A:243:ILE:CD1	1:C:243:ILE:HD11	2.46	0.45
1:J:9:LEU:HD13	1:J:89:LEU:HG	1.98	0.45
1:I:87:ASP:HB3	1:I:197:GLU:OE1	2.16	0.45
1:C:50:ARG:HD3	1:C:263:PHE:CZ	2.51	0.45
1:I:227:THR:HG23	1:I:233:LEU:HA	1.99	0.45
1:L:177:TYR:CD1	1:L:177:TYR:N	2.84	0.45
1:J:142:ASP:HB2	1:J:145:ARG:HG3	1.99	0.45
1:I:31:ILE:HB	1:I:39:TYR:CE1	2.52	0.45
1:A:31:ILE:HB	1:A:39:TYR:CE1	2.51	0.45
1:B:50:ARG:HD3	1:B:263:PHE:CE1	2.52	0.45
1:D:150:GLU:O	1:D:158:VAL:HG22	2.17	0.45
1:B:195:ARG:O	1:B:197:GLU:HG2	2.16	0.44
1:J:152:ASP:HB3	1:J:156:THR:H	1.82	0.44
1:J:31:ILE:HB	1:J:39:TYR:CE1	2.52	0.44
1:A:7:ILE:HG12	1:A:53:LEU:HB3	2.00	0.44
1:K:177:TYR:N	1:K:177:TYR:CD1	2.84	0.44
1:B:89:LEU:HB3	1:B:200:ILE:HD11	1.98	0.44
1:J:177:TYR:N	1:J:177:TYR:CD1	2.86	0.44
1:B:227:THR:HG23	1:B:233:LEU:HA	2.00	0.44
1:L:143:PRO:CG	1:L:170:ASN:HA	2.47	0.44
1:B:171:TYR:CE1	1:B:217:MET:HG3	2.52	0.44
1:C:171:TYR:CE1	1:C:217:MET:HG3	2.52	0.44
1:I:142:ASP:HB2	1:I:145:ARG:HG3	1.99	0.44
2:K:500:DTP:O2G	2:K:500:DTP:O2B	2.33	0.44
1:A:17:LEU:HD12	1:A:26:LYS:HD3	1.98	0.44
1:J:260:ARG:NH1	1:J:260:ARG:CG	2.81	0.44
1:A:227:THR:CG2	1:A:233:LEU:HD13	2.47	0.44
1:J:208:MET:HB2	1:J:213:LEU:HD23	2.00	0.44
1:J:192:PRO:HB3	1:J:197:GLU:N	2.32	0.44
1:K:31:ILE:HB	1:K:39:TYR:CE1	2.53	0.44
1:D:137:ALA:HB1	1:D:171:TYR:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG12	1:C:53:LEU:HB3	1.99	0.44
1:J:87:ASP:HB3	1:J:197:GLU:OE1	2.16	0.44
1:I:208:MET:HB2	1:I:213:LEU:HD23	2.00	0.44
1:L:171:TYR:CE1	1:L:217:MET:HG3	2.53	0.44
1:J:239:PHE:CD1	1:L:246:ARG:HG3	2.52	0.44
1:C:137:ALA:HB1	1:C:171:TYR:HB3	1.99	0.43
1:D:142:ASP:OD1	1:D:142:ASP:N	2.51	0.43
1:K:31:ILE:HD11	1:K:227:THR:HG21	2.01	0.43
1:D:210:GLN:OE1	1:D:212:ARG:NH1	2.52	0.43
1:L:152:ASP:HB3	1:L:156:THR:H	1.83	0.43
1:L:208:MET:HB2	1:L:213:LEU:HD23	1.99	0.43
1:L:137:ALA:HB1	1:L:171:TYR:HB3	2.00	0.43
1:C:17:LEU:HD12	1:C:26:LYS:HD3	2.00	0.43
1:A:132:GLY:HA2	1:A:207:TYR:CE2	2.53	0.43
1:A:9:LEU:HD13	1:A:89:LEU:HG	2.00	0.43
1:A:276:LEU:O	1:A:282:GLY:HA3	2.18	0.43
1:L:122:LEU:HD22	1:L:222:TYR:OH	2.19	0.43
1:K:142:ASP:OD1	1:K:142:ASP:N	2.51	0.43
1:C:142:ASP:OD1	1:C:142:ASP:N	2.51	0.43
1:J:249:LEU:HD22	1:J:249:LEU:O	2.18	0.43
1:B:142:ASP:N	1:B:142:ASP:OD1	2.52	0.43
1:K:74:TRP:HE1	1:K:255:GLU:HG3	1.83	0.43
1:C:19:PRO:HD2	1:D:33:ASP:O	2.19	0.43
1:J:150:GLU:O	1:J:158:VAL:HG22	2.19	0.43
1:B:177:TYR:CD1	1:B:177:TYR:N	2.87	0.43
1:L:142:ASP:HB2	1:L:145:ARG:HG3	2.00	0.43
1:D:112:ASN:HB3	1:D:114:PHE:CE1	2.53	0.43
1:K:112:ASN:HB3	1:K:114:PHE:CE1	2.54	0.43
1:B:210:GLN:OE1	1:B:212:ARG:NH1	2.52	0.43
1:C:132:GLY:HA3	1:C:212:ARG:HB3	2.01	0.43
1:B:9:LEU:HG	1:B:107:LEU:HD11	2.00	0.43
1:B:220:ARG:NH1	1:D:284:TYR:OH	2.52	0.43
1:A:165:LEU:O	1:A:167:PRO:HD3	2.18	0.43
1:B:150:GLU:O	1:B:158:VAL:HG22	2.17	0.43
1:L:227:THR:CG2	1:L:233:LEU:HD13	2.49	0.43
1:B:144:GLU:HG2	1:B:145:ARG:HG2	2.01	0.43
1:L:112:ASN:HB3	1:L:114:PHE:CE1	2.54	0.43
1:D:249:LEU:HD22	1:D:249:LEU:O	2.19	0.43
1:D:165:LEU:HA	1:D:165:LEU:HD12	1.89	0.43
1:B:205:ARG:O	1:B:208:MET:N	2.52	0.42
1:A:192:PRO:HB3	1:A:197:GLU:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:PRO:HB3	1:K:197:GLU:N	2.34	0.42
1:I:192:PRO:HB3	1:I:197:GLU:N	2.34	0.42
1:C:9:LEU:HD13	1:C:89:LEU:HG	2.02	0.42
1:K:137:ALA:HB1	1:K:171:TYR:HB3	2.00	0.42
1:I:142:ASP:N	1:I:142:ASP:OD1	2.49	0.42
1:B:34:LYS:HE2	1:B:251:VAL:O	2.19	0.42
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.90	0.42
1:K:195:ARG:O	1:K:197:GLU:HG2	2.20	0.42
1:I:152:ASP:HB3	1:I:156:THR:H	1.84	0.42
1:K:150:GLU:O	1:K:158:VAL:HG22	2.19	0.42
1:L:74:TRP:NE1	1:L:255:GLU:HG3	2.35	0.42
1:J:227:THR:CG2	1:J:233:LEU:HD13	2.50	0.42
1:B:31:ILE:HB	1:B:39:TYR:CE1	2.55	0.42
1:A:150:GLU:O	1:A:158:VAL:HG22	2.19	0.42
1:B:205:ARG:CD	1:B:208:MET:CE	2.94	0.42
1:L:263:PHE:N	1:L:263:PHE:CD2	2.88	0.42
1:D:61:THR:O	1:D:65:GLN:HG3	2.19	0.42
1:A:152:ASP:HB3	1:A:156:THR:H	1.84	0.42
1:L:249:LEU:C	1:L:249:LEU:HD12	2.40	0.42
1:L:144:GLU:HG2	1:L:145:ARG:HG2	2.00	0.42
1:B:112:ASN:HB3	1:B:114:PHE:CE1	2.55	0.42
1:L:31:ILE:HB	1:L:39:TYR:CE1	2.55	0.42
1:B:9:LEU:HD13	1:B:89:LEU:HD13	2.01	0.42
1:A:108:VAL:HA	1:A:175:GLY:O	2.19	0.42
1:K:165:LEU:HA	1:K:165:LEU:HD12	1.89	0.42
1:B:71:GLY:HA3	1:B:78:LEU:HG	2.02	0.42
1:A:74:TRP:NE1	1:A:255:GLU:HG3	2.35	0.42
1:J:137:ALA:HB1	1:J:171:TYR:HB3	2.02	0.41
1:K:119:LEU:HB3	1:K:120:PRO:HD3	2.02	0.41
1:B:7:ILE:HG12	1:B:53:LEU:HB3	2.02	0.41
1:K:278:LYS:HD3	1:L:15:THR:OG1	2.20	0.41
1:J:220:ARG:NH1	1:L:284:TYR:CZ	2.88	0.41
1:D:31:ILE:HD11	1:D:227:THR:HG21	2.03	0.41
1:J:31:ILE:HD11	1:J:227:THR:HG21	2.02	0.41
1:K:142:ASP:HB2	1:K:145:ARG:HG3	2.01	0.41
1:J:269:VAL:HG11	1:J:289:VAL:CG1	2.50	0.41
1:I:7:ILE:HG12	1:I:53:LEU:HB3	2.01	0.41
1:A:165:LEU:C	1:A:167:PRO:HD3	2.41	0.41
1:A:195:ARG:O	1:A:197:GLU:HG2	2.21	0.41
1:J:227:THR:HG23	1:J:233:LEU:HA	2.02	0.41
1:D:74:TRP:NE1	1:D:255:GLU:HG3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:ARG:NH1	1:I:260:ARG:CG	2.81	0.41
1:I:247:GLN:HA	1:K:222:TYR:O	2.20	0.41
1:I:31:ILE:HD11	1:I:227:THR:HG21	2.03	0.41
1:K:74:TRP:NE1	1:K:255:GLU:HG3	2.35	0.41
1:D:119:LEU:HB3	1:D:120:PRO:HD3	2.02	0.41
1:L:210:GLN:OE1	1:L:212:ARG:NH1	2.53	0.41
1:B:152:ASP:HB3	1:B:156:THR:H	1.85	0.41
1:J:132:GLY:HA2	1:J:207:TYR:HE2	1.84	0.41
1:A:137:ALA:HB1	1:A:171:TYR:HB3	2.01	0.41
1:K:164:PRO:CG	1:K:167:PRO:HA	2.51	0.41
1:K:210:GLN:OE1	1:K:212:ARG:NH1	2.54	0.41
1:C:112:ASN:HB3	1:C:114:PHE:CE1	2.55	0.41
1:C:119:LEU:HB3	1:C:120:PRO:HD3	2.02	0.41
1:B:142:ASP:HB2	1:B:145:ARG:HG3	2.03	0.41
1:J:50:ARG:HD3	1:J:263:PHE:CZ	2.56	0.41
1:L:61:THR:N	1:L:62:PRO:CD	2.84	0.41
1:C:108:VAL:HA	1:C:175:GLY:O	2.21	0.41
1:B:198:LEU:CD1	1:B:198:LEU:N	2.73	0.41
1:L:31:ILE:HD11	1:L:227:THR:HG21	2.02	0.41
1:I:137:ALA:HB1	1:I:171:TYR:HB3	2.02	0.41
1:I:74:TRP:HE1	1:I:255:GLU:HG3	1.86	0.41
1:B:263:PHE:CD2	1:B:263:PHE:N	2.88	0.41
1:I:177:TYR:CD1	1:I:177:TYR:N	2.88	0.41
1:L:165:LEU:O	1:L:167:PRO:HD3	2.21	0.41
1:J:7:ILE:HG12	1:J:53:LEU:HB3	2.03	0.41
1:B:196:GLY:HA2	1:J:65:GLN:OE1	2.21	0.40
1:D:152:ASP:HB3	1:D:156:THR:H	1.86	0.40
1:J:132:GLY:HA3	1:J:212:ARG:HB3	2.03	0.40
1:D:108:VAL:HA	1:D:175:GLY:O	2.21	0.40
1:L:142:ASP:OD1	1:L:142:ASP:N	2.54	0.40
1:K:243:ILE:HA	1:K:243:ILE:HD13	1.88	0.40
1:L:165:LEU:HA	1:L:165:LEU:HD12	1.92	0.40
1:J:2:LYS:O	1:J:2:LYS:HG2	2.21	0.40
1:J:263:PHE:N	1:J:263:PHE:CD2	2.90	0.40
1:C:165:LEU:HA	1:C:165:LEU:HD12	1.92	0.40
1:C:61:THR:O	1:C:65:GLN:HG3	2.22	0.40
1:I:119:LEU:HB3	1:I:120:PRO:HD3	2.03	0.40
1:J:144:GLU:HG2	1:J:145:ARG:HG2	2.03	0.40
1:D:89:LEU:HB3	1:D:200:ILE:HD11	2.03	0.40
1:I:112:ASN:HB3	1:I:114:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

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	
1	A	288/292 (99%)	280 (97%)	8 (3%)	0	100	100
1	B	287/292 (98%)	278 (97%)	9 (3%)	0	100	100
1	C	278/292 (95%)	273 (98%)	5 (2%)	0	100	100
1	D	279/292 (96%)	273 (98%)	6 (2%)	0	100	100
1	I	287/292 (98%)	279 (97%)	8 (3%)	0	100	100
1	J	287/292 (98%)	278 (97%)	8 (3%)	1 (0%)	46	72
1	K	280/292 (96%)	274 (98%)	6 (2%)	0	100	100
1	L	280/292 (96%)	275 (98%)	5 (2%)	0	100	100
All	All	2266/2336 (97%)	2210 (98%)	55 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	289	VAL

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	
1	A	244/245 (100%)	234 (96%)	10 (4%)	37	66
1	B	243/245 (99%)	235 (97%)	8 (3%)	45	73
1	C	238/245 (97%)	232 (98%)	6 (2%)	55	81
1	D	239/245 (98%)	232 (97%)	7 (3%)	50	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	243/245 (99%)	235 (97%)	8 (3%)	45	73
1	J	243/245 (99%)	232 (96%)	11 (4%)	34	62
1	K	239/245 (98%)	230 (96%)	9 (4%)	40	68
1	L	240/245 (98%)	235 (98%)	5 (2%)	61	85
All	All	1929/1960 (98%)	1865 (97%)	64 (3%)	45	73

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	145	ARG
1	A	165	LEU
1	A	169	SER
1	A	195	ARG
1	A	197	GLU
1	A	198	LEU
1	A	225	LEU
1	A	281	TYR
1	A	290	LYS
1	B	145	ARG
1	B	169	SER
1	B	190	LEU
1	B	195	ARG
1	B	197	GLU
1	B	205	ARG
1	B	281	TYR
1	B	290	LYS
1	C	122	LEU
1	C	169	SER
1	C	190	LEU
1	C	197	GLU
1	C	281	TYR
1	C	290	LYS
1	D	122	LEU
1	D	145	ARG
1	D	169	SER
1	D	197	GLU
1	D	225	LEU
1	D	249	LEU
1	D	290	LYS
1	I	91	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	145	ARG
1	I	169	SER
1	I	195	ARG
1	I	197	GLU
1	I	225	LEU
1	I	281	TYR
1	I	290	LYS
1	J	107	LEU
1	J	122	LEU
1	J	145	ARG
1	J	160	LEU
1	J	169	SER
1	J	195	ARG
1	J	197	GLU
1	J	203	ILE
1	J	225	LEU
1	J	249	LEU
1	J	281	TYR
1	K	107	LEU
1	K	122	LEU
1	K	135	VAL
1	K	169	SER
1	K	177	TYR
1	K	195	ARG
1	K	197	GLU
1	K	198	LEU
1	K	290	LYS
1	L	122	LEU
1	L	145	ARG
1	L	169	SER
1	L	197	GLU
1	L	290	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\# Z > 2$
2	DTP	A	500	3	24,32,32	1.02	1 (4%)	32,50,50	1.87	5 (15%)
2	DTP	B	500	3	24,32,32	1.16	2 (8%)	32,50,50	1.97	5 (15%)
2	DTP	C	500	3	24,32,32	1.08	2 (8%)	32,50,50	3.64	9 (28%)
2	DTP	D	500	3	24,32,32	1.02	1 (4%)	32,50,50	1.91	5 (15%)
2	DTP	I	500	3	24,32,32	1.09	2 (8%)	32,50,50	2.14	7 (21%)
2	DTP	J	500	3	24,32,32	1.06	2 (8%)	32,50,50	3.63	9 (28%)
2	DTP	K	500	3	24,32,32	1.09	2 (8%)	32,50,50	3.27	7 (21%)
2	DTP	L	500	3	24,32,32	1.10	1 (4%)	32,50,50	1.94	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	A	500	3	-	0/18/34/34	0/3/3/3
2	DTP	B	500	3	-	0/18/34/34	0/3/3/3
2	DTP	C	500	3	-	0/18/34/34	0/3/3/3
2	DTP	D	500	3	-	0/18/34/34	0/3/3/3
2	DTP	I	500	3	-	0/18/34/34	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	J	500	3	-	0/18/34/34	0/3/3/3
2	DTP	K	500	3	-	0/18/34/34	0/3/3/3
2	DTP	L	500	3	-	0/18/34/34	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	DTP	PG-O2G	-2.67	1.45	1.54
2	K	500	DTP	PG-O3G	-2.32	1.46	1.54
2	B	500	DTP	PG-O2G	-2.16	1.47	1.54
2	J	500	DTP	PG-O2G	-2.05	1.47	1.54
2	I	500	DTP	PB-O1B	2.11	1.58	1.51
2	D	500	DTP	C5-C4	3.11	1.47	1.40
2	C	500	DTP	C5-C4	3.18	1.47	1.40
2	I	500	DTP	C5-C4	3.19	1.47	1.40
2	K	500	DTP	C5-C4	3.38	1.48	1.40
2	J	500	DTP	C5-C4	3.39	1.48	1.40
2	L	500	DTP	C5-C4	3.52	1.48	1.40
2	A	500	DTP	C5-C4	3.60	1.48	1.40
2	B	500	DTP	C5-C4	3.62	1.48	1.40

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	DTP	O2G-PG-O3B	-7.64	70.45	105.09
2	B	500	DTP	N3-C2-N1	-7.39	123.24	128.89
2	J	500	DTP	O2G-PG-O3B	-7.22	72.33	105.09
2	I	500	DTP	N3-C2-N1	-6.60	123.84	128.89
2	C	500	DTP	N3-C2-N1	-6.38	124.01	128.89
2	J	500	DTP	N3-C2-N1	-6.32	124.05	128.89
2	K	500	DTP	N3-C2-N1	-6.29	124.08	128.89
2	D	500	DTP	N3-C2-N1	-6.27	124.09	128.89
2	A	500	DTP	N3-C2-N1	-6.09	124.23	128.89
2	L	500	DTP	N3-C2-N1	-5.97	124.32	128.89
2	C	500	DTP	O3G-PG-O2G	-5.90	84.90	107.38
2	K	500	DTP	O2G-PG-O3B	-5.80	78.76	105.09
2	J	500	DTP	O3G-PG-O1G	-5.30	93.51	110.58
2	L	500	DTP	PA-O3A-PB	-5.11	118.38	132.73
2	J	500	DTP	O3G-PG-O2G	-4.87	88.85	107.38
2	I	500	DTP	PA-O3A-PB	-4.57	119.90	132.73
2	C	500	DTP	O3G-PG-O1G	-3.84	98.23	110.58
2	D	500	DTP	PA-O3A-PB	-3.71	122.30	132.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	DTP	PA-O3A-PB	-3.66	122.45	132.73
2	A	500	DTP	PA-O3A-PB	-3.55	122.75	132.73
2	L	500	DTP	C4-C5-N7	-3.53	106.23	109.48
2	K	500	DTP	O3G-PG-O1G	-3.51	99.30	110.58
2	I	500	DTP	C4-C5-N7	-3.24	106.50	109.48
2	C	500	DTP	C4-C5-N7	-3.21	106.53	109.48
2	J	500	DTP	PA-O3A-PB	-3.18	123.80	132.73
2	K	500	DTP	C4-C5-N7	-3.15	106.58	109.48
2	C	500	DTP	PA-O3A-PB	-3.06	124.14	132.73
2	J	500	DTP	C4-C5-N7	-2.92	106.79	109.48
2	D	500	DTP	C4-C5-N7	-2.90	106.81	109.48
2	K	500	DTP	PA-O3A-PB	-2.90	124.59	132.73
2	I	500	DTP	O2G-PG-O3B	-2.89	91.96	105.09
2	D	500	DTP	O2G-PG-O3B	-2.58	93.37	105.09
2	B	500	DTP	C4-C5-N7	-2.45	107.23	109.48
2	B	500	DTP	O2G-PG-O3B	-2.42	94.10	105.09
2	A	500	DTP	O2G-PG-O3B	-2.36	94.37	105.09
2	I	500	DTP	O2B-PB-O3B	-2.36	94.39	105.09
2	L	500	DTP	O2G-PG-O3B	-2.35	94.44	105.09
2	A	500	DTP	C4-C5-N7	-2.12	107.53	109.48
2	J	500	DTP	O2B-PB-O3B	2.02	114.26	105.09
2	C	500	DTP	O2B-PB-O3B	2.10	114.60	105.09
2	C	500	DTP	O3G-PG-O3B	2.17	114.96	105.09
2	J	500	DTP	O3G-PG-O3B	2.20	115.07	105.09
2	L	500	DTP	O3G-PG-O3B	2.26	115.33	105.09
2	K	500	DTP	O2B-PB-O3B	2.26	115.34	105.09
2	B	500	DTP	O2G-PG-O1G	3.78	122.76	110.58
2	L	500	DTP	O2G-PG-O1G	3.94	123.26	110.58
2	I	500	DTP	O2B-PB-O1B	4.07	134.56	112.53
2	D	500	DTP	O2G-PG-O1G	4.85	126.21	110.58
2	I	500	DTP	O2G-PG-O1G	5.02	126.74	110.58
2	A	500	DTP	O2G-PG-O1G	5.44	128.11	110.58
2	K	500	DTP	O2G-PG-O1G	14.57	157.47	110.58
2	J	500	DTP	O2G-PG-O1G	15.13	159.30	110.58
2	C	500	DTP	O2G-PG-O1G	15.20	159.51	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	DTP	1	0
2	J	500	DTP	1	0
2	K	500	DTP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	290/292 (99%)	-0.14	4 (1%) 78 74	28, 58, 116, 148	0
1	B	289/292 (98%)	-0.08	5 (1%) 73 68	32, 64, 120, 161	0
1	C	282/292 (96%)	0.17	14 (4%) 32 26	37, 84, 128, 160	0
1	D	283/292 (96%)	0.36	23 (8%) 15 10	40, 89, 137, 165	0
1	I	289/292 (98%)	-0.15	3 (1%) 84 81	35, 64, 117, 148	0
1	J	289/292 (98%)	0.05	9 (3%) 52 45	35, 64, 124, 163	0
1	K	284/292 (97%)	0.69	42 (14%) 3 2	55, 104, 147, 205	0
1	L	284/292 (97%)	0.60	36 (12%) 5 3	51, 100, 144, 165	0
All	All	2290/2336 (98%)	0.18	136 (5%) 26 19	28, 81, 133, 205	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	193	SER	8.2
1	K	194	ALA	7.8
1	L	211	GLY	6.4
1	L	210	GLN	6.2
1	L	208	MET	6.1
1	J	196	GLY	5.4
1	L	158	VAL	5.2
1	K	289	VAL	5.1
1	D	289	VAL	5.1
1	C	154	LYS	5.0
1	K	275	PRO	4.9
1	L	209	GLU	4.8
1	K	84	PRO	4.8
1	L	212	ARG	4.7
1	K	198	LEU	4.6
1	D	190	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	158	VAL	4.4
1	K	276	LEU	4.3
1	L	214	SER	4.1
1	L	154	LYS	4.0
1	K	190	LEU	3.9
1	K	102	HIS	3.9
1	K	157	ALA	3.9
1	L	213	LEU	3.9
1	J	192	PRO	3.8
1	K	204	ASN	3.8
1	L	153	GLN	3.8
1	C	158	VAL	3.7
1	L	127	VAL	3.7
1	D	187	ALA	3.7
1	L	129	LYS	3.7
1	L	2	LYS	3.6
1	D	209	GLU	3.5
1	L	152	ASP	3.5
1	K	154	LYS	3.5
1	K	262	ASN	3.5
1	L	157	ALA	3.4
1	C	155	GLY	3.4
1	D	208	MET	3.4
1	D	3	THR	3.4
1	J	157	ALA	3.4
1	C	152	ASP	3.4
1	K	151	PHE	3.3
1	C	170	ASN	3.3
1	K	166	GLN	3.3
1	K	103	ASP	3.3
1	L	94	ILE	3.3
1	D	189	ASN	3.3
1	K	208	MET	3.2
1	K	214	SER	3.2
1	J	212	ARG	3.2
1	L	160	LEU	3.1
1	K	197	GLU	3.1
1	L	215	VAL	3.0
1	D	204	ASN	2.9
1	B	161	GLU	2.9
1	K	134	THR	2.9
1	L	205	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	168	LYS	2.9
1	C	157	ALA	2.9
1	K	209	GLU	2.9
1	D	264	ILE	2.9
1	D	211	GLY	2.9
1	K	93	PHE	2.8
1	K	169	SER	2.8
1	L	190	LEU	2.8
1	L	150	GLU	2.7
1	C	153	GLN	2.7
1	K	213	LEU	2.7
1	J	152	ASP	2.7
1	B	157	ALA	2.7
1	C	3	THR	2.7
1	L	207	TYR	2.7
1	D	5	LYS	2.7
1	K	264	ILE	2.7
1	B	130	GLU	2.6
1	D	130	GLU	2.6
1	A	1	MET	2.6
1	D	186	MET	2.6
1	L	131	SER	2.6
1	C	84	PRO	2.6
1	L	99	PHE	2.6
1	C	128	ASN	2.6
1	K	94	ILE	2.6
1	K	272	LEU	2.6
1	D	269	VAL	2.6
1	K	268	GLN	2.5
1	K	215	VAL	2.5
1	I	154	LYS	2.4
1	K	192	PRO	2.4
1	K	210	GLN	2.4
1	K	271	GLU	2.4
1	L	290	LYS	2.4
1	D	213	LEU	2.3
1	L	133	ALA	2.3
1	B	151	PHE	2.3
1	K	196	GLY	2.3
1	L	3	THR	2.3
1	J	154	LYS	2.3
1	D	159	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	154	LYS	2.3
1	L	189	ASN	2.3
1	K	155	GLY	2.3
1	K	212	ARG	2.3
1	K	186	MET	2.3
1	L	186	MET	2.3
1	I	157	ALA	2.3
1	K	126	ALA	2.3
1	B	192	PRO	2.3
1	J	149	VAL	2.2
1	A	161	GLU	2.2
1	K	285	LEU	2.2
1	L	171	TYR	2.2
1	D	191	LYS	2.2
1	J	290	LYS	2.2
1	D	210	GLN	2.2
1	C	150	GLU	2.2
1	C	156	THR	2.2
1	D	185	GLU	2.2
1	L	206	ILE	2.1
1	D	168	LYS	2.1
1	L	197	GLU	2.1
1	C	151	PHE	2.1
1	A	220	ARG	2.1
1	K	170	ASN	2.1
1	J	195	ARG	2.1
1	L	156	THR	2.1
1	L	89	LEU	2.1
1	D	212	ARG	2.1
1	C	4	ARG	2.1
1	L	126	ALA	2.1
1	I	130	GLU	2.0
1	L	22	MET	2.0
1	K	203	ILE	2.0
1	D	290	LYS	2.0
1	K	91	GLN	2.0

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

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
2	DTP	K	500	30/30	0.91	0.23	0.72	51,106,138,154	30
2	DTP	L	500	30/30	0.91	0.18	0.25	66,96,128,142	0
2	DTP	B	500	30/30	0.95	0.15	0.11	33,68,101,113	0
2	DTP	I	500	30/30	0.98	0.14	-0.54	34,67,110,133	0
2	DTP	A	500	30/30	0.97	0.15	-0.56	38,67,106,141	0
2	DTP	J	500	30/30	0.97	0.15	-0.57	34,66,106,156	0
2	DTP	C	500	30/30	0.96	0.14	-0.58	42,83,110,146	0
2	DTP	D	500	30/30	0.98	0.14	-0.78	55,79,110,121	0
3	MG	K	502	1/1	0.89	0.26	-	30,30,30,30	0
3	MG	B	501	1/1	0.83	0.19	-	50,50,50,50	0
3	MG	J	501	1/1	0.96	0.29	-	69,69,69,69	0
3	MG	L	502	1/1	0.89	0.19	-	68,68,68,68	0
3	MG	I	501	1/1	0.89	0.13	-	64,64,64,64	0
3	MG	C	502	1/1	0.85	0.18	-	61,61,61,61	0
3	MG	D	502	1/1	0.88	0.18	-	66,66,66,66	0
3	MG	L	501	1/1	0.73	0.19	-	69,69,69,69	0
3	MG	C	501	1/1	0.67	0.33	-	61,61,61,61	0
3	MG	K	501	1/1	0.54	0.28	-	30,30,30,30	0
3	MG	I	502	1/1	0.97	0.23	-	55,55,55,55	0
3	MG	J	502	1/1	0.98	0.20	-	57,57,57,57	0
3	MG	D	501	1/1	0.66	0.21	-	67,67,67,67	0
3	MG	A	501	1/1	0.83	0.28	-	61,61,61,61	0
3	MG	A	502	1/1	0.93	0.27	-	53,53,53,53	0
3	MG	B	502	1/1	0.94	0.18	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.