



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:06 AM GMT

PDB ID : 2ZI5  
Title : C4S dCK variant of dCK in complex with L-dA+UDP  
Authors : Sabini, E.; Lavie, A.  
Deposited on : 2008-02-13  
Resolution : 1.77 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](mailto: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.

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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

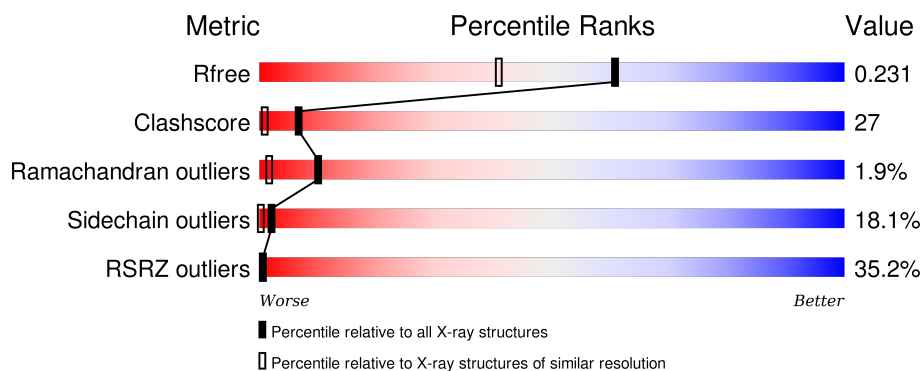
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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  $\geq 3$ , 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	279	<div> <div>29%</div> <div> <div>33%</div> <div>34%</div> <div>11%</div> <div>22%</div> </div> </div>
1	B	279	<div> <div>24%</div> <div> <div>39%</div> <div>32%</div> <div>9%</div> <div>20%</div> </div> </div>
1	C	279	<div> <div>31%</div> <div> <div>33%</div> <div>35%</div> <div>10%</div> <div>22%</div> </div> </div>
1	D	279	<div> <div>28%</div> <div> <div>39%</div> <div>33%</div> <div>6%</div> <div>22%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7716 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	2	0
			1837	1184	304	343	6			
1	B	223	Total	C	N	O	S	0	3	0
			1856	1197	308	345	6			
1	C	219	Total	C	N	O	S	0	3	0
			1827	1176	304	341	6			
1	D	218	Total	C	N	O	S	0	1	0
			1813	1170	298	339	6			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	982	MET	-	EXPRESSION TAG	UNP P27707
A	983	GLY	-	EXPRESSION TAG	UNP P27707
A	984	SER	-	EXPRESSION TAG	UNP P27707
A	985	SER	-	EXPRESSION TAG	UNP P27707
A	986	HIS	-	EXPRESSION TAG	UNP P27707
A	987	HIS	-	EXPRESSION TAG	UNP P27707
A	988	HIS	-	EXPRESSION TAG	UNP P27707
A	989	HIS	-	EXPRESSION TAG	UNP P27707
A	990	HIS	-	EXPRESSION TAG	UNP P27707
A	991	HIS	-	EXPRESSION TAG	UNP P27707
A	992	SER	-	EXPRESSION TAG	UNP P27707
A	993	GLY	-	EXPRESSION TAG	UNP P27707
A	994	LEU	-	EXPRESSION TAG	UNP P27707
A	995	VAL	-	EXPRESSION TAG	UNP P27707
A	996	PRO	-	EXPRESSION TAG	UNP P27707
A	997	ARG	-	EXPRESSION TAG	UNP P27707
A	998	GLY	-	EXPRESSION TAG	UNP P27707
A	999	SER	-	EXPRESSION TAG	UNP P27707
A	1000	HIS	-	EXPRESSION TAG	UNP P27707
A	1009	SER	CYS	ENGINEERED	UNP P27707
A	1045	SER	CYS	ENGINEERED	UNP P27707

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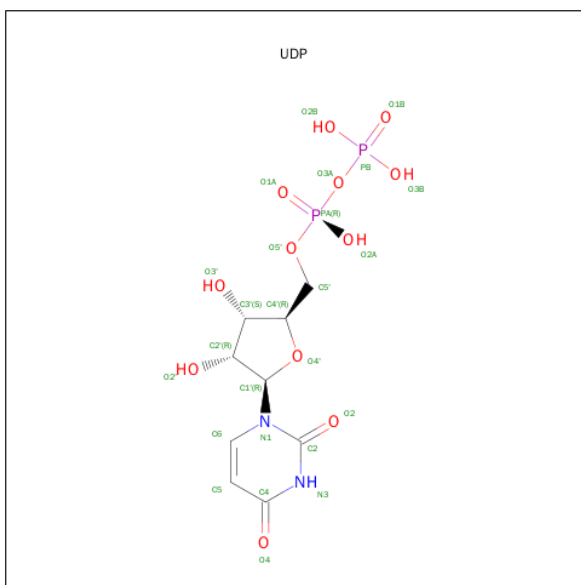
Chain	Residue	Modelled	Actual	Comment	Reference
A	1059	SER	CYS	ENGINEERED	UNP P27707
A	1146	SER	CYS	ENGINEERED	UNP P27707
B	1982	MET	-	EXPRESSION TAG	UNP P27707
B	1983	GLY	-	EXPRESSION TAG	UNP P27707
B	1984	SER	-	EXPRESSION TAG	UNP P27707
B	1985	SER	-	EXPRESSION TAG	UNP P27707
B	1986	HIS	-	EXPRESSION TAG	UNP P27707
B	1987	HIS	-	EXPRESSION TAG	UNP P27707
B	1988	HIS	-	EXPRESSION TAG	UNP P27707
B	1989	HIS	-	EXPRESSION TAG	UNP P27707
B	1990	HIS	-	EXPRESSION TAG	UNP P27707
B	1991	HIS	-	EXPRESSION TAG	UNP P27707
B	1992	SER	-	EXPRESSION TAG	UNP P27707
B	1993	GLY	-	EXPRESSION TAG	UNP P27707
B	1994	LEU	-	EXPRESSION TAG	UNP P27707
B	1995	VAL	-	EXPRESSION TAG	UNP P27707
B	1996	PRO	-	EXPRESSION TAG	UNP P27707
B	1997	ARG	-	EXPRESSION TAG	UNP P27707
B	1998	GLY	-	EXPRESSION TAG	UNP P27707
B	1999	SER	-	EXPRESSION TAG	UNP P27707
B	2000	HIS	-	EXPRESSION TAG	UNP P27707
B	2009	SER	CYS	ENGINEERED	UNP P27707
B	2045	SER	CYS	ENGINEERED	UNP P27707
B	2059	SER	CYS	ENGINEERED	UNP P27707
B	2146	SER	CYS	ENGINEERED	UNP P27707
C	2982	MET	-	EXPRESSION TAG	UNP P27707
C	2983	GLY	-	EXPRESSION TAG	UNP P27707
C	2984	SER	-	EXPRESSION TAG	UNP P27707
C	2985	SER	-	EXPRESSION TAG	UNP P27707
C	2986	HIS	-	EXPRESSION TAG	UNP P27707
C	2987	HIS	-	EXPRESSION TAG	UNP P27707
C	2988	HIS	-	EXPRESSION TAG	UNP P27707
C	2989	HIS	-	EXPRESSION TAG	UNP P27707
C	2990	HIS	-	EXPRESSION TAG	UNP P27707
C	2991	HIS	-	EXPRESSION TAG	UNP P27707
C	2992	SER	-	EXPRESSION TAG	UNP P27707
C	2993	GLY	-	EXPRESSION TAG	UNP P27707
C	2994	LEU	-	EXPRESSION TAG	UNP P27707
C	2995	VAL	-	EXPRESSION TAG	UNP P27707
C	2996	PRO	-	EXPRESSION TAG	UNP P27707
C	2997	ARG	-	EXPRESSION TAG	UNP P27707
C	2998	GLY	-	EXPRESSION TAG	UNP P27707

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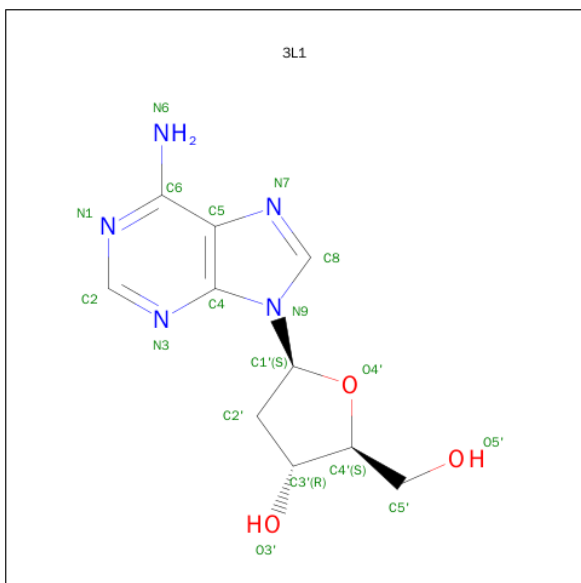
Chain	Residue	Modelled	Actual	Comment	Reference
C	2999	SER	-	EXPRESSION TAG	UNP P27707
C	3000	HIS	-	EXPRESSION TAG	UNP P27707
C	3009	SER	CYS	ENGINEERED	UNP P27707
C	3045	SER	CYS	ENGINEERED	UNP P27707
C	3059	SER	CYS	ENGINEERED	UNP P27707
C	3146	SER	CYS	ENGINEERED	UNP P27707
D	3982	MET	-	EXPRESSION TAG	UNP P27707
D	3983	GLY	-	EXPRESSION TAG	UNP P27707
D	3984	SER	-	EXPRESSION TAG	UNP P27707
D	3985	SER	-	EXPRESSION TAG	UNP P27707
D	3986	HIS	-	EXPRESSION TAG	UNP P27707
D	3987	HIS	-	EXPRESSION TAG	UNP P27707
D	3988	HIS	-	EXPRESSION TAG	UNP P27707
D	3989	HIS	-	EXPRESSION TAG	UNP P27707
D	3990	HIS	-	EXPRESSION TAG	UNP P27707
D	3991	HIS	-	EXPRESSION TAG	UNP P27707
D	3992	SER	-	EXPRESSION TAG	UNP P27707
D	3993	GLY	-	EXPRESSION TAG	UNP P27707
D	3994	LEU	-	EXPRESSION TAG	UNP P27707
D	3995	VAL	-	EXPRESSION TAG	UNP P27707
D	3996	PRO	-	EXPRESSION TAG	UNP P27707
D	3997	ARG	-	EXPRESSION TAG	UNP P27707
D	3998	GLY	-	EXPRESSION TAG	UNP P27707
D	3999	SER	-	EXPRESSION TAG	UNP P27707
D	4000	HIS	-	EXPRESSION TAG	UNP P27707
D	4009	SER	CYS	ENGINEERED	UNP P27707
D	4045	SER	CYS	ENGINEERED	UNP P27707
D	4059	SER	CYS	ENGINEERED	UNP P27707
D	4146	SER	CYS	ENGINEERED	UNP P27707

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	B	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	C	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	D	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 3 is (2S,3R,5S)-5-(6-AMINO-9H-PURIN-9-YL)-TETRAHYDRO-2-(HYDROXY METHYL)FURAN-3-OL (three-letter code: 3L1) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	10	5	3		
3	B	1	Total	C	N	O	0	0
			18	10	5	3		
3	C	1	Total	C	N	O	0	0
			18	10	5	3		
3	D	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 4 is water.

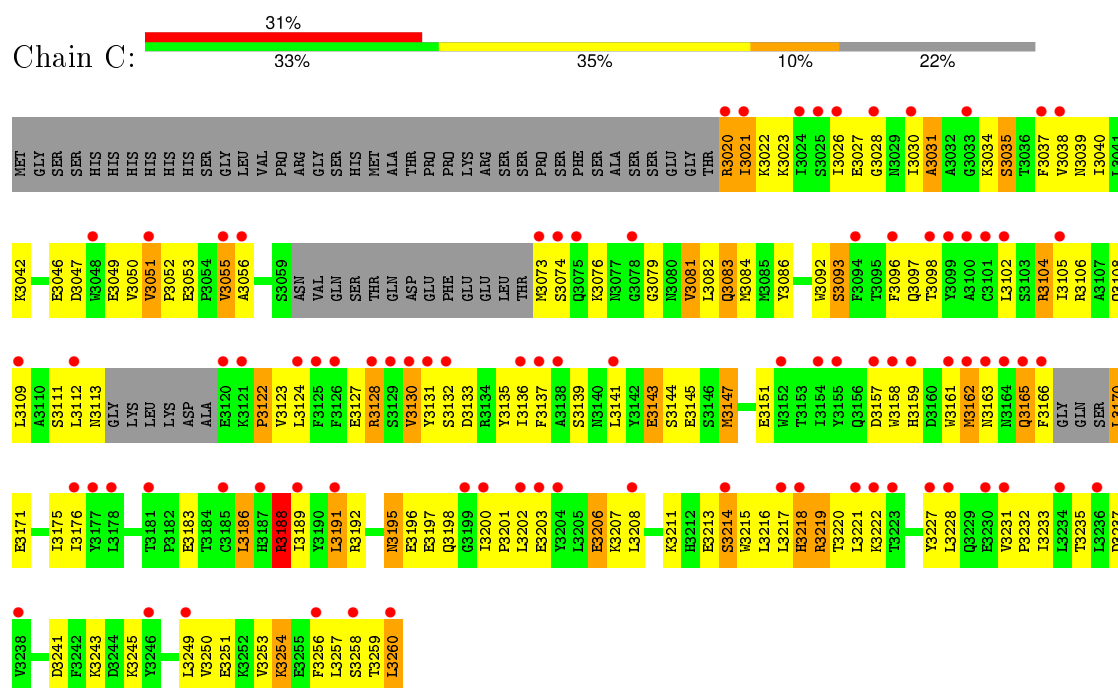
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	71	Total	O	0	0
			71	71		
4	C	62	Total	O	0	0
			62	62		
4	D	35	Total	O	0	0
			35	35		



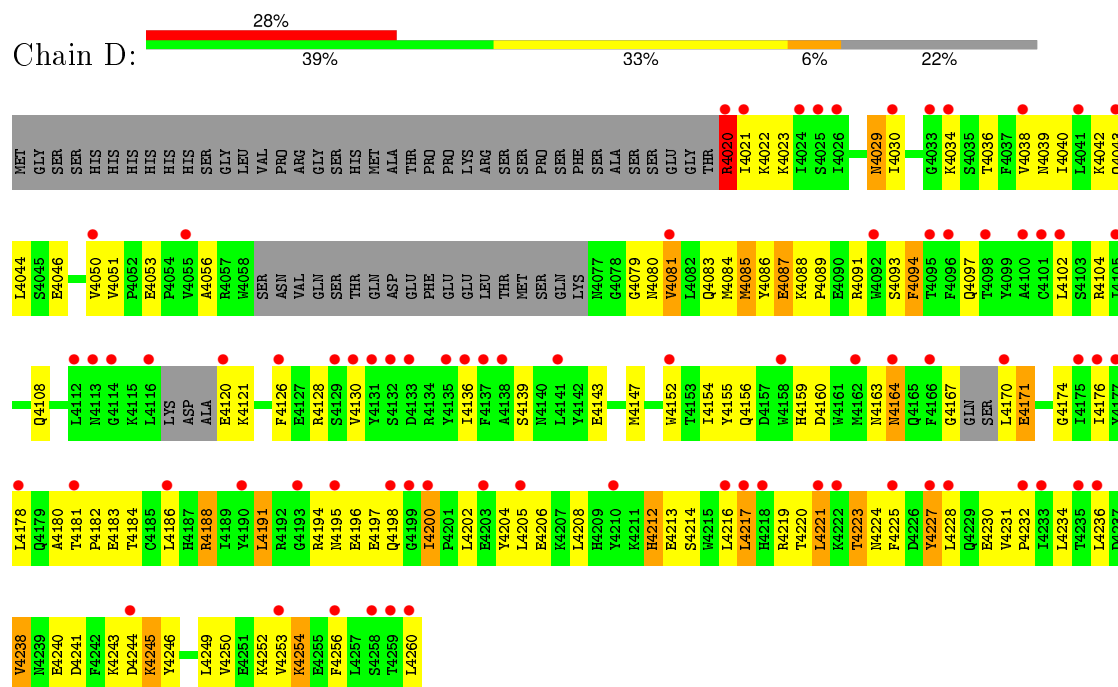




- Molecule 1: Deoxycytidine kinase



- Molecule 1: Deoxycytidine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.36Å 138.65Å 119.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.77 29.95 – 1.77	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.77) 93.7 (29.95-1.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.77Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.219 , 0.293 0.230 , 0.231	Depositor DCC
$R_{free}$ test set	10496 reflections (11.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 76.9	EDS
Estimated twinning fraction	0.477 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 110723 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	7716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.70 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5149e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: UDP, 3L1

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	0.36	0/1888	1.04	1/2556 (0.0%)
1	B	0.38	0/1907	1.13	8/2581 (0.3%)
1	C	0.36	0/1875	1.05	7/2537 (0.3%)
1	D	0.37	0/1859	1.14	12/2516 (0.5%)
All	All	0.37	0/7529	1.09	28/10190 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2128	ARG	NE-CZ-NH1	-12.30	114.15	120.30
1	D	4020	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	D	4155	TYR	CB-CG-CD2	8.90	126.34	121.00
1	D	4020	ARG	CD-NE-CZ	8.90	136.06	123.60
1	B	2128	ARG	CD-NE-CZ	-8.35	111.92	123.60
1	B	2134	ARG	CD-NE-CZ	7.93	134.70	123.60
1	D	4094	PHE	CZ-CE2-CD2	-7.53	111.07	120.10
1	A	1177	TYR	CB-CG-CD1	7.19	125.31	121.00
1	D	4155	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	D	4094	PHE	CB-CG-CD1	-6.44	116.29	120.80
1	D	4094	PHE	CG-CD1-CE1	-6.36	113.80	120.80
1	C	3188	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	3128	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	3104	ARG	CD-NE-CZ	6.02	132.03	123.60
1	D	4188	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	2128	ARG	NH1-CZ-NH2	5.62	125.58	119.40
1	D	4212	HIS	CA-CB-CG	5.57	123.07	113.60
1	B	2219	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	4188	ARG	CD-NE-CZ	5.33	131.06	123.60
1	C	3104	ARG	NE-CZ-NH1	5.32	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2134	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	3188	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	2134	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	3237	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	4188	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	2152	TRP	CA-CB-CG	5.09	123.37	113.70
1	D	4147	MET	CA-CB-CG	5.06	121.90	113.30
1	C	3218	HIS	C-N-CA	5.00	134.20	121.70

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	1837	0	1779	108	0
1	B	1856	0	1818	100	0
1	C	1827	0	1766	108	0
1	D	1813	0	1752	92	0
2	A	25	0	11	2	0
2	B	25	0	11	0	0
2	C	25	0	11	3	0
2	D	25	0	11	4	0
3	A	18	0	13	2	0
3	B	18	0	13	0	0
3	C	18	0	13	2	0
3	D	18	0	13	1	0
4	A	43	0	0	5	0
4	B	71	0	0	7	0
4	C	62	0	0	7	0
4	D	35	0	0	2	0
All	All	7716	0	7211	399	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 27.

All (399) 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:2203:GLU:O	4:B:6066:HOH:O	1.56	1.17
1:A:1046[B]:GLU:CD	1:A:1046[B]:GLU:H	1.52	1.08
1:A:1081:VAL:HA	1:A:1084:MET:HE2	1.43	1.00
1:D:4194:ARG:HB2	1:D:4197:GLU:HG3	1.45	0.97
1:A:1038:VAL:HG13	1:A:1050:VAL:HG11	1.49	0.92
1:A:1186:LEU:HA	1:A:1189:ILE:HG13	1.49	0.91
1:D:4221:LEU:HD23	1:D:4223:THR:HG22	1.54	0.90
1:C:3031:ALA:HB1	1:C:3188:ARG:HB3	1.53	0.87
1:A:1056:ALA:O	4:A:6137:HOH:O	1.91	0.87
1:D:4036:THR:HG21	1:D:4243:LYS:HE2	1.61	0.83
1:C:3109:LEU:HA	1:C:3112:LEU:HD12	1.61	0.82
1:D:4234:LEU:HD21	1:D:4236:LEU:HD21	1.63	0.80
1:B:2075:GLN:HE21	1:B:2075:GLN:HA	1.48	0.79
1:D:4202:LEU:O	1:D:4206:GLU:HG3	1.83	0.79
1:B:2116:LEU:HB3	1:B:2122:PRO:HB3	1.66	0.76
1:C:3111:SER:OG	1:C:3124:LEU:HD21	1.85	0.76
1:B:2039:ASN:OD1	1:B:2042:LYS:HE3	1.84	0.76
1:D:4225:PHE:HB2	1:D:4228:LEU:HD12	1.68	0.75
1:D:4178:LEU:HB3	1:D:4238:VAL:HG11	1.66	0.74
1:D:4139:SER:O	1:D:4143:GLU:HG3	1.86	0.74
1:C:3162:MET:O	1:C:3165[B]:GLN:HB3	1.88	0.73
1:A:1225:PHE:O	1:A:1228:LEU:HB2	1.87	0.73
1:A:1187:HIS:O	1:A:1191:LEU:HD13	1.89	0.73
1:C:3162:MET:O	1:C:3165[A]:GLN:HB2	1.88	0.73
1:B:2177:TYR:HD2	1:B:2235:THR:HG1	1.37	0.73
1:A:1055:VAL:HG23	4:A:6177:HOH:O	1.88	0.73
1:A:1134:ARG:HD3	1:A:1159:HIS:ND1	2.05	0.72
1:A:1181:THR:HG23	1:A:1239:ASN:HD21	1.55	0.72
1:D:4053:GLU:OE1	1:D:4128:ARG:HD2	1.89	0.71
1:C:3108:GLN:HB3	1:C:3170:LEU:HD11	1.72	0.70
1:D:4160:ASP:O	1:D:4164:ASN:HB2	1.92	0.70
1:A:1130:VAL:HG21	1:A:1163:ASN:ND2	2.05	0.70
1:D:4167:GLY:O	1:D:4171:GLU:HB2	1.92	0.69
1:A:1150:THR:O	1:A:1154:ILE:HG13	1.93	0.69
1:A:1105:ILE:HD11	1:A:1163:ASN:OD1	1.93	0.68
1:D:4079:GLY:O	1:D:4083:GLN:HG2	1.92	0.68
1:C:3213:GLU:OE2	1:C:3217:LEU:HD22	1.91	0.68
1:A:1045:SER:C	1:A:1046[B]:GLU:OE1	2.31	0.68
1:A:1080:ASN:ND2	1:C:3245:LYS:HG3	2.09	0.68
1:C:3030:ILE:HD11	3:C:3401:3L1:H2'	1.76	0.68
1:C:3232:PRO:HG3	1:C:3260:LEU:HD22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2083:GLN:OE1	1:D:4245:LYS:HE2	1.93	0.68
1:B:2104:ARG:O	1:B:2108:GLN:HG3	1.93	0.67
1:C:3186:LEU:HD12	1:C:3202:LEU:HD13	1.77	0.67
1:D:4180:ALA:HB2	1:D:4238:VAL:HG22	1.75	0.67
1:A:1188:ARG:HA	1:A:1191:LEU:HB2	1.77	0.67
1:C:3147:MET:HG2	1:C:3151:GLU:HB3	1.77	0.67
1:B:2102:LEU:HD11	1:B:2106:ARG:HD2	1.77	0.66
1:C:3251:GLU:HA	1:C:3251:GLU:OE2	1.96	0.66
1:A:1027:GLU:OE1	4:A:6180:HOH:O	2.13	0.66
1:C:3202:LEU:HG	1:C:3206:GLU:OE2	1.96	0.65
1:B:2147:MET:HG2	1:B:2151:GLU:HB2	1.78	0.65
1:B:2047:ASP:HB3	1:B:2121:LYS:O	1.97	0.64
1:A:1080:ASN:O	1:A:1084:MET:HG3	1.98	0.64
1:D:4195:ASN:HA	1:D:4198:GLN:HG2	1.79	0.64
1:B:2021:ILE:HG12	1:B:2122:PRO:HB2	1.78	0.64
1:A:1052:PRO:HA	1:A:1127:GLU:HB2	1.79	0.63
1:C:3133:ASP:HB3	4:C:6086:HOH:O	1.96	0.63
1:C:3021:ILE:HG23	1:C:3122:PRO:HB2	1.80	0.63
1:B:2076:LYS:NZ	1:D:4244:ASP:HB3	2.14	0.63
1:D:4038:VAL:HG22	1:D:4050:VAL:HG22	1.80	0.62
1:B:2053:GLU:HG3	1:B:2104:ARG:HH12	1.64	0.62
1:C:3093:SER:OG	1:C:3141:LEU:HD13	2.00	0.62
1:C:3098:THR:HG23	1:C:3158:TRP:CE2	2.35	0.62
1:D:4197:GLU:O	1:D:4200:ILE:HG13	2.00	0.61
1:D:4040:ILE:HA	1:D:4043:GLN:OE1	2.01	0.61
1:B:2026:ILE:HD11	1:B:2125:PHE:HB3	1.83	0.61
1:A:1023:LYS:HD2	1:A:1171:GLU:O	2.00	0.61
1:C:3197:GLU:O	1:C:3200:ILE:HG13	2.00	0.61
1:B:2060:ASN:HD22	1:B:2194:ARG:HE	1.49	0.61
1:B:2221:LEU:O	1:B:2222:LYS:HE3	2.00	0.60
1:C:3218:HIS:O	1:C:3220:THR:HG23	2.02	0.60
1:A:1204:TYR:CZ	1:A:1208:LEU:HD11	2.36	0.60
1:B:2177:TYR:HE2	1:B:2217:LEU:HD22	1.66	0.60
1:A:1086:TYR:CE1	1:A:1196:GLU:HG3	2.37	0.60
1:C:3052:PRO:HB3	4:C:6013:HOH:O	2.01	0.60
1:C:3022:LYS:HZ1	1:C:3260:LEU:HB2	1.67	0.59
1:B:2171:GLU:HG2	1:B:2227:TYR:CZ	2.36	0.59
1:D:4152:TRP:O	1:D:4156:GLN:HG3	2.02	0.59
1:A:1204:TYR:O	1:A:1207:LYS:HB2	2.02	0.59
1:C:3104:ARG:HH12	1:C:3128:ARG:HB2	1.68	0.59
1:B:2186:LEU:HD22	1:B:2202:LEU:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2116:LEU:HB3	1:B:2122:PRO:CB	2.33	0.59
1:D:4020:ARG:HB2	1:D:4020:ARG:HH11	1.68	0.59
1:C:3123:VAL:HG21	1:C:3257:LEU:HD13	1.84	0.59
1:D:4159:HIS:O	1:D:4163:ASN:HB2	2.03	0.58
1:C:3175:ILE:HD12	1:C:3231:VAL:HG11	1.85	0.58
1:C:3081:VAL:HG13	1:C:3096:PHE:HD1	1.67	0.58
1:A:1177:TYR:CE2	1:A:1179:GLN:HG3	2.39	0.58
1:D:4040:ILE:HD13	1:D:4246:TYR:CD2	2.37	0.58
1:C:3214:SER:HA	1:C:3218:HIS:CD2	2.39	0.58
1:C:3215:TRP:CD1	1:C:3221:LEU:HD23	2.39	0.58
1:B:2109:LEU:CD2	1:B:2170:LEU:HD11	2.33	0.58
1:C:3102:LEU:O	1:C:3105:ILE:HB	2.04	0.58
1:B:2105:ILE:O	1:B:2109:LEU:HG	2.03	0.58
1:D:4093:SER:O	1:D:4097:GLN:HB2	2.03	0.58
1:C:3165[A]:GLN:HA	1:C:3165[A]:GLN:HE21	1.69	0.58
1:A:1049:GLU:HB2	1:A:1124:LEU:CD1	2.34	0.57
1:C:3022:LYS:NZ	1:C:3260:LEU:HB2	2.20	0.57
1:B:2026:ILE:CD1	1:B:2125:PHE:HB3	2.34	0.57
1:D:4250:VAL:HG12	1:D:4254:LYS:HE3	1.87	0.57
1:B:2221:LEU:HD12	1:B:2222:LYS:H	1.69	0.57
1:A:1094:PHE:CE2	1:B:2095:THR:HG23	2.40	0.57
1:C:3139:SER:OG	1:C:3211:LYS:HE3	2.05	0.56
1:A:1102:LEU:HG	1:A:1102:LEU:O	2.03	0.56
1:B:2041:LEU:HB3	1:B:2048:TRP:CZ3	2.40	0.56
1:D:4180:ALA:HB2	1:D:4238:VAL:CG2	2.36	0.56
1:A:1112:LEU:HD21	1:A:1169:SER:O	2.05	0.56
1:B:2022:LYS:HA	1:B:2173:ASP:OD2	2.06	0.56
1:C:3073:MET:O	1:C:3076:LYS:HB3	2.06	0.56
1:A:1194:ARG:HB3	1:A:1197:GLU:HG3	1.89	0.55
1:A:1236:LEU:HD13	1:A:1249:LEU:HD22	1.87	0.55
1:A:1087:GLU:OE2	1:A:1087:GLU:HA	2.07	0.55
1:B:2101:CYS:HB3	1:B:2158:TRP:HH2	1.71	0.55
1:A:1185:CYS:O	1:A:1189:ILE:HG12	2.07	0.54
1:A:1196:GLU:HG2	1:A:1197:GLU:N	2.23	0.54
1:A:1051:VAL:HG13	1:A:1126:PHE:HD2	1.72	0.54
1:A:1200:ILE:HG21	1:A:1205:LEU:HD21	1.90	0.54
1:A:1041:LEU:O	1:A:1048:TRP:HE3	1.90	0.54
1:B:2108:GLN:HB3	1:B:2126:PHE:CE2	2.43	0.54
1:D:4108:GLN:OE1	1:D:4170:LEU:HD13	2.08	0.54
1:D:4174:GLY:HA2	1:D:4231:VAL:HG22	1.89	0.54
1:B:2250:VAL:HG12	4:B:6071:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3053:GLU:O	1:C:3056:ALA:HB3	2.08	0.54
1:C:3144:SER:O	1:C:3145:GLU:HB2	2.08	0.54
1:B:2054:PRO:HG2	4:B:6028:HOH:O	2.08	0.54
1:A:1053:GLU:HB3	1:A:1127:GLU:O	2.08	0.54
1:B:2034:LYS:O	1:B:2038:VAL:HB	2.08	0.54
1:C:3227:TYR:CE2	1:C:3228:LEU:HG	2.43	0.54
1:C:3028:GLY:N	1:C:3034:LYS:HD3	2.22	0.54
1:A:1135:TYR:O	1:A:1136:ILE:HD13	2.07	0.54
1:A:1153:THR:CG2	1:B:2077:ASN:HD21	2.20	0.54
1:C:3055:VAL:HG11	3:C:3401:3L1:N3	2.24	0.53
1:C:3035:SER:HB2	2:C:3301:UDP:O1B	2.08	0.53
1:B:2195:ASN:N	1:B:2195:ASN:HD22	2.04	0.53
1:B:2049:GLU:HG3	4:B:6055:HOH:O	2.07	0.53
1:B:2221:LEU:HD12	1:B:2222:LYS:N	2.24	0.53
1:A:1158:TRP:CZ2	1:A:1162:MET:HG2	2.43	0.53
1:A:1112:LEU:HD12	1:A:1112:LEU:O	2.07	0.53
1:D:4083:GLN:O	1:D:4087[A]:GLU:HB2	2.08	0.53
1:D:4130:VAL:HG11	1:D:4163:ASN:HD21	1.72	0.53
1:D:4088:LYS:HD3	1:D:4091:ARG:CB	2.39	0.53
1:D:4167:GLY:HA2	1:D:4171:GLU:OE2	2.09	0.53
1:A:1080:ASN:HD22	1:C:3245:LYS:HG3	1.74	0.53
1:B:2030:ILE:O	1:B:2185:CYS:HB3	2.08	0.53
1:B:2109:LEU:HD21	1:B:2170:LEU:HD11	1.91	0.53
1:B:2026:ILE:HD13	1:B:2038:VAL:CG2	2.39	0.52
1:A:1190:TYR:HD2	1:A:1198:GLN:HE22	1.57	0.52
1:D:4182:PRO:HB2	1:D:4202:LEU:HD11	1.90	0.52
1:A:1181:THR:HG23	1:A:1239:ASN:ND2	2.22	0.52
1:B:2108:GLN:HB2	1:B:2170:LEU:HD22	1.90	0.52
1:C:3161:TRP:O	1:C:3165[A]:GLN:HG2	2.08	0.52
1:B:2041:LEU:HD23	1:B:2250:VAL:HG22	1.92	0.52
1:D:4085:MET:CE	1:D:4089:PRO:HB3	2.40	0.52
1:C:3165[A]:GLN:NE2	1:C:3165[A]:GLN:HA	2.25	0.52
1:A:1023:LYS:HD3	1:A:1169:SER:O	2.09	0.52
1:C:3195:ASN:HA	1:C:3198:GLN:HG2	1.91	0.52
1:C:3175:ILE:CD1	1:C:3231:VAL:HG11	2.40	0.52
1:C:3038:VAL:HG22	1:C:3050:VAL:CG2	2.39	0.52
1:D:4230:GLU:O	1:D:4232:PRO:HD3	2.10	0.51
1:A:1153:THR:HG21	1:B:2077:ASN:HD21	1.75	0.51
1:C:3135:TYR:HB3	1:C:3221:LEU:HD21	1.92	0.51
1:A:1086:TYR:OH	3:A:1401:3L1:H4'	2.10	0.51
1:D:4081:VAL:HA	1:D:4084:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2134:ARG:HD3	1:B:2159:HIS:CE1	2.45	0.51
1:D:4198:GLN:HG3	4:D:6113:HOH:O	2.09	0.51
1:C:3109:LEU:CD2	1:C:3170:LEU:HD12	2.41	0.50
1:A:1112:LEU:HD23	1:A:1170:LEU:HD23	1.93	0.50
1:A:1130:VAL:HG11	1:A:1163:ASN:OD1	2.10	0.50
1:D:4087[B]:GLU:HA	1:D:4087[B]:GLU:OE1	2.11	0.50
3:D:4401:3L1:H8	3:D:4401:3L1:O5'	2.11	0.50
1:B:2134:ARG:HD3	1:B:2159:HIS:ND1	2.25	0.50
1:C:3202:LEU:O	1:C:3206:GLU:OE2	2.29	0.50
1:D:4223:THR:HG1	1:D:4225:PHE:HD1	1.58	0.50
1:C:3027:GLU:OE2	1:C:3132:SER:OG	2.30	0.50
1:D:4088:LYS:HD3	1:D:4091:ARG:HB3	1.93	0.50
1:C:3051:VAL:O	1:C:3051:VAL:HG22	2.11	0.50
1:C:3112:LEU:HD11	1:C:3170:LEU:HG	1.93	0.50
1:A:1131:TYR:CG	1:A:1228:LEU:HD11	2.46	0.50
1:A:1203:GLU:HA	1:A:1206:GLU:HG3	1.94	0.50
1:C:3098:THR:HG23	1:C:3158:TRP:CZ2	2.47	0.50
1:C:3035:SER:HB3	2:C:3301:UDP:O2A	2.12	0.50
1:A:1049:GLU:HB2	1:A:1124:LEU:HD12	1.93	0.49
1:B:2041:LEU:HB3	1:B:2048:TRP:CE3	2.47	0.49
1:A:1021:ILE:HG22	1:A:1021:ILE:O	2.11	0.49
1:D:4194:ARG:HB3	1:D:4196:GLU:OE2	2.12	0.49
1:C:3022:LYS:NZ	1:C:3260:LEU:HD12	2.26	0.49
1:D:4160:ASP:OD1	1:D:4224:ASN:OD1	2.30	0.49
1:A:1200:ILE:O	1:A:1200:ILE:HG22	2.11	0.49
1:A:1082:LEU:HA	1:A:1096:PHE:CE1	2.48	0.49
1:B:2147:MET:HG2	1:B:2151:GLU:CB	2.42	0.49
1:A:1241:ASP:OD1	2:A:1301:UDP:O4	2.30	0.49
1:B:2236:LEU:CD2	1:B:2252:LYS:HD2	2.41	0.49
1:C:3139:SER:O	1:C:3143:GLU:OE1	2.30	0.49
1:C:3136:ILE:HG23	1:C:3208:LEU:HD22	1.93	0.49
1:B:2177:TYR:CE2	1:B:2217:LEU:HD22	2.46	0.49
1:D:4130:VAL:HG21	1:D:4163:ASN:ND2	2.27	0.49
1:B:2206:GLU:HB2	4:B:6066:HOH:O	2.13	0.49
1:A:1047:ASP:HB3	1:A:1121:LYS:O	2.13	0.49
1:C:3256:PHE:O	1:C:3259:THR:OG1	2.29	0.49
1:A:1053:GLU:H	1:A:1127:GLU:HB3	1.78	0.49
1:C:3055:VAL:HG12	4:C:6173:HOH:O	2.12	0.49
1:B:2041:LEU:CD2	1:B:2250:VAL:HG22	2.43	0.48
1:C:3031:ALA:CB	1:C:3188:ARG:HB3	2.33	0.48
1:A:1194:ARG:O	1:A:1198:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2149:GLU:O	1:B:2153:THR:OG1	2.29	0.48
1:A:1053:GLU:HA	1:A:1054:PRO:HD3	1.63	0.48
1:D:4053:GLU:O	1:D:4056:ALA:HB3	2.13	0.48
1:B:2037:PHE:O	1:B:2040:ILE:HB	2.14	0.48
1:B:2053:GLU:HG3	1:B:2104:ARG:NH1	2.29	0.48
1:D:4036:THR:CG2	1:D:4243:LYS:HE2	2.40	0.48
1:C:3197:GLU:HB3	1:C:3200:ILE:HD12	1.95	0.48
1:B:2051[A]:VAL:HG23	4:B:6003:HOH:O	2.13	0.48
1:D:4136:ILE:HG22	1:D:4208:LEU:HD22	1.96	0.48
1:A:1046[B]:GLU:OE1	1:A:1046[B]:GLU:CA	2.58	0.48
1:A:1037:PHE:CE2	1:A:1041:LEU:HD11	2.49	0.48
1:C:3081:VAL:HG13	1:C:3096:PHE:CD1	2.48	0.47
1:A:1024:ILE:HG21	1:A:1176:ILE:HD12	1.96	0.47
1:A:1250:VAL:HG12	1:A:1254:LYS:HD2	1.95	0.47
1:D:4256:PHE:O	1:D:4260:LEU:HG	2.14	0.47
1:D:4243:LYS:HE3	2:D:4301:UDP:N1	2.29	0.47
1:A:1134:ARG:CZ	1:A:1156:GLN:HG2	2.44	0.47
1:A:1111[A]:SER:HB3	1:A:1124:LEU:HD21	1.96	0.47
1:A:1054:PRO:CA	1:A:1057:ARG:HH21	2.27	0.47
1:B:2058:TRP:HD1	1:B:2075:GLN:NE2	2.12	0.47
1:D:4038:VAL:HG22	1:D:4050:VAL:CG2	2.42	0.47
1:A:1157:ASP:O	1:A:1160:ASP:HB2	2.14	0.47
1:D:4038:VAL:HG21	1:D:4050:VAL:HG13	1.95	0.47
1:C:3038:VAL:HG22	1:C:3050:VAL:HG22	1.96	0.47
1:C:3076:LYS:HE2	4:C:6092:HOH:O	2.14	0.47
1:A:1162:MET:O	1:A:1166:PHE:HD2	1.97	0.47
1:B:2250:VAL:O	1:B:2254:LYS:HG3	2.15	0.47
1:A:1054:PRO:HG3	1:A:1057:ARG:HH21	1.80	0.47
1:B:2076:LYS:HZ2	1:D:4244:ASP:HB3	1.80	0.47
1:D:4040:ILE:O	1:D:4044:LEU:HG	2.15	0.47
1:D:4234:LEU:CD2	1:D:4236:LEU:HD21	2.39	0.46
1:C:3232:PRO:CG	1:C:3260:LEU:HD22	2.43	0.46
1:B:2042:LYS:HG2	1:B:2043:GLN:N	2.30	0.46
1:C:3076:LYS:HA	4:C:6043:HOH:O	2.15	0.46
1:C:3131:TYR:CG	1:C:3228:LEU:HD11	2.50	0.46
1:C:3192:ARG:HB3	4:C:6094:HOH:O	2.16	0.46
1:D:4088:LYS:O	1:D:4088:LYS:HG2	2.14	0.46
1:A:1084:MET:HE3	1:A:1092:TRP:CD2	2.50	0.46
1:B:2234:LEU:HB2	1:B:2256:PHE:CD2	2.50	0.46
1:D:4221:LEU:HD23	1:D:4223:THR:CG2	2.37	0.46
1:A:1038:VAL:CG1	1:A:1050:VAL:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4223:THR:HG1	1:D:4225:PHE:H	1.60	0.46
1:B:2198:GLN:OE1	1:B:2198:GLN:HA	2.16	0.46
1:A:1158:TRP:O	1:A:1162:MET:N	2.49	0.46
1:C:3249:LEU:O	1:C:3253:VAL:HG23	2.16	0.46
1:A:1052:PRO:HA	1:A:1127:GLU:CB	2.44	0.46
1:C:3191:LEU:HD23	1:C:3191:LEU:HA	1.73	0.45
1:D:4249:LEU:HD23	1:D:4249:LEU:N	2.31	0.45
1:B:2207:LYS:N	4:B:6066:HOH:O	2.49	0.45
1:D:4029:ASN:O	1:D:4034:LYS:NZ	2.50	0.45
1:A:1250:VAL:O	1:A:1254:LYS:HD2	2.15	0.45
1:D:4213:GLU:O	1:D:4217:LEU:HB3	2.15	0.45
1:B:2177:TYR:CE2	1:B:2179:GLN:HG3	2.51	0.45
1:A:1029:ASN:O	1:A:1034:LYS:NZ	2.50	0.45
1:B:2076:LYS:HZ3	1:D:4244:ASP:HB3	1.80	0.45
1:A:1192:ARG:NH2	1:A:1197:GLU:OE1	2.50	0.45
1:A:1241:ASP:CG	2:A:1301:UDP:HN3	2.19	0.45
1:B:2208:LEU:N	1:B:2208:LEU:HD23	2.31	0.45
1:A:1188:ARG:NH2	1:A:1238:VAL:O	2.50	0.45
1:B:2108:GLN:HB2	1:B:2170:LEU:CD2	2.46	0.45
1:C:3250:VAL:O	1:C:3254:LYS:HG3	2.17	0.45
1:D:4195:ASN:ND2	4:D:6113:HOH:O	2.49	0.45
1:B:2109:LEU:HD23	1:B:2170:LEU:HD11	1.98	0.45
1:C:3136:ILE:CG2	1:C:3208:LEU:HD22	2.46	0.45
1:C:3147:MET:CG	1:C:3151:GLU:HB3	2.46	0.45
1:C:3200:ILE:HA	1:C:3201:PRO:HD3	1.84	0.45
1:C:3128:ARG:NH2	4:C:6215:HOH:O	2.49	0.45
1:C:3026:ILE:HG22	1:C:3034:LYS:HG2	1.99	0.45
1:D:4212:HIS:HB3	1:D:4216:LEU:HD12	1.99	0.45
1:B:2053:GLU:OE1	1:B:2128:ARG:HD2	2.17	0.45
1:C:3127:GLU:O	1:C:3128:ARG:HB2	2.16	0.45
1:B:2091:ARG:HG3	1:B:2091:ARG:HH11	1.82	0.45
1:D:4023:LYS:HB2	1:D:4023:LYS:HE3	1.61	0.45
1:A:1145:GLU:HA	4:A:6102:HOH:O	2.16	0.45
1:B:2235:THR:HG22	1:B:2235:THR:O	2.16	0.45
1:D:4080:ASN:HA	1:D:4083:GLN:HG2	1.98	0.45
1:C:3104:ARG:NH1	1:C:3128:ARG:HB2	2.31	0.45
1:C:3219:ARG:NH1	1:C:3233:ILE:HD12	2.32	0.45
1:A:1203:GLU:H	1:A:1203:GLU:CD	2.20	0.45
1:B:2197:GLU:HB3	1:B:2200:ILE:HD12	1.98	0.44
1:D:4167:GLY:C	1:D:4171:GLU:HB2	2.36	0.44
1:C:3220:THR:OG1	1:C:3220:THR:O	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2223:THR:OG1	1:B:2229:GLN:NE2	2.49	0.44
1:C:3111:SER:HG	1:C:3124:LEU:HD21	1.77	0.44
1:A:1167:GLY:O	1:A:1169:SER:N	2.50	0.44
1:B:2194:ARG:O	1:B:2198:GLN:NE2	2.50	0.44
1:B:2177:TYR:HD2	1:B:2235:THR:OG1	1.99	0.44
1:A:1204:TYR:O	1:A:1207:LYS:N	2.50	0.44
1:C:3130:VAL:HB	1:C:3159:HIS:NE2	2.32	0.44
1:A:1106:ARG:NH1	1:B:2157:ASP:OD2	2.50	0.44
1:D:4194:ARG:CB	1:D:4197:GLU:HG3	2.33	0.44
1:B:2171:GLU:HG2	1:B:2227:TYR:CE2	2.51	0.44
1:A:1183:GLU:OE2	1:A:1183:GLU:N	2.50	0.44
1:D:4034:LYS:NZ	2:D:4301:UDP:O3B	2.51	0.44
1:A:1201:PRO:HB3	1:A:1203:GLU:OE1	2.18	0.44
1:C:3084:MET:HB3	1:C:3092:TRP:NE1	2.33	0.44
1:D:4188:ARG:O	1:D:4191:LEU:HB2	2.18	0.44
1:C:3020:ARG:NE	1:C:3122:PRO:HG2	2.32	0.44
1:A:1047:ASP:HA	1:A:1119:ALA:CB	2.48	0.44
1:D:4204:TYR:CZ	1:D:4208:LEU:HD11	2.52	0.43
1:A:1022:LYS:HZ2	1:A:1123:VAL:HG22	1.83	0.43
1:A:1052:PRO:HG2	1:A:1057:ARG:HH12	1.83	0.43
1:D:4188:ARG:HG2	2:D:4301:UDP:O4'	2.17	0.43
1:D:4224:ASN:O	1:D:4224:ASN:ND2	2.51	0.43
1:D:4171:GLU:HG3	1:D:4227:TYR:CZ	2.52	0.43
1:C:3082:LEU:HD11	1:C:3086:TYR:HE1	1.83	0.43
1:B:2075:GLN:O	1:B:2079:GLY:N	2.50	0.43
1:C:3213:GLU:CD	1:C:3217:LEU:HD22	2.38	0.43
1:C:3192:ARG:NH1	2:C:3301:UDP:O1A	2.50	0.43
1:A:1209:HIS:O	1:A:1212:HIS:N	2.49	0.43
1:A:1196:GLU:N	1:A:1196:GLU:OE1	2.50	0.43
1:C:3027:GLU:C	1:C:3034:LYS:HD3	2.39	0.43
1:C:3165[B]:GLN:O	1:C:3165[B]:GLN:HG3	2.17	0.43
1:B:2051[A]:VAL:HG22	1:B:2126:PHE:HD2	1.84	0.43
1:A:1023:LYS:NZ	1:A:1171:GLU:O	2.49	0.43
1:A:1037:PHE:CD2	1:A:1041:LEU:HD11	2.53	0.43
1:B:2080:ASN:O	1:B:2084:MET:HG3	2.19	0.43
1:D:4051:VAL:HG13	1:D:4126:PHE:HD2	1.84	0.43
1:B:2215:TRP:HZ2	1:B:2228:LEU:HD11	1.82	0.43
1:A:1171:GLU:HG2	1:A:1227:TYR:CZ	2.53	0.42
1:B:2194:ARG:HD3	1:B:2197:GLU:OE2	2.19	0.42
1:C:3105:ILE:HG22	1:C:3106:ARG:N	2.34	0.42
4:A:6064:HOH:O	1:B:2094:PHE:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:PRO:O	1:A:1057:ARG:NH2	2.50	0.42
1:D:4243:LYS:HE3	2:D:4301:UDP:C2	2.55	0.42
1:D:4240:GLU:CD	1:D:4245:LYS:HE3	2.39	0.42
1:A:1051:VAL:O	1:A:1051:VAL:HG22	2.20	0.42
1:B:2148:ASN:OD1	1:B:2150:THR:HB	2.19	0.42
1:D:4085:MET:HE3	1:D:4089:PRO:HB3	2.00	0.42
1:C:3037:PHE:O	1:C:3040:ILE:HB	2.20	0.42
1:D:4094:PHE:CE1	1:D:4154:ILE:HG22	2.54	0.42
1:B:2255:GLU:O	1:B:2258:SER:N	2.50	0.42
1:D:4196:GLU:H	1:D:4196:GLU:CD	2.23	0.42
1:B:2047:ASP:OD2	1:B:2121:LYS:N	2.50	0.42
1:C:3171:GLU:HB3	1:C:3227:TYR:CZ	2.55	0.42
1:A:1161:TRP:CZ2	1:A:1165:GLN:HG3	2.55	0.42
1:B:2116:LEU:N	1:B:2116:LEU:HD23	2.34	0.42
1:A:1053:GLU:O	1:A:1056:ALA:HB3	2.20	0.42
1:C:3030:ILE:CG2	1:C:3189:ILE:HD11	2.50	0.42
1:A:1026:ILE:HD13	1:A:1176:ILE:HB	2.01	0.42
1:B:2053:GLU:H	1:B:2127:GLU:HB3	1.84	0.42
1:C:3175:ILE:HB	1:C:3233:ILE:HG12	2.00	0.42
1:B:2131:TYR:CE1	1:B:2172:LEU:HD11	2.55	0.42
1:D:4080:ASN:O	1:D:4083:GLN:HG3	2.20	0.41
1:B:2102:LEU:CD1	1:B:2106:ARG:HD2	2.48	0.41
1:C:3132:SER:O	1:C:3136:ILE:HB	2.20	0.41
1:B:2114:GLY:O	1:B:2115:LYS:HE2	2.20	0.41
1:C:3079:GLY:O	1:C:3083:GLN:HB2	2.19	0.41
1:B:2081:VAL:HA	1:B:2084:MET:HG3	2.02	0.41
1:B:2090:GLU:H	1:B:2090:GLU:CD	2.23	0.41
1:C:3097:GLN:HE21	1:C:3141:LEU:HD11	1.85	0.41
1:A:1218:HIS:O	1:A:1219:ARG:HB2	2.19	0.41
1:C:3213:GLU:O	1:C:3217:LEU:HB3	2.20	0.41
1:A:1047:ASP:OD2	1:A:1119:ALA:HB1	2.21	0.41
1:D:4029:ASN:OD1	1:D:4030:ILE:N	2.50	0.41
1:C:3021:ILE:HG22	1:C:3022:LYS:N	2.35	0.41
1:C:3136:ILE:HG22	1:C:3137:PHE:N	2.36	0.41
1:D:4085:MET:HE1	1:D:4089:PRO:HB3	2.02	0.41
1:A:1241:ASP:OD1	1:A:1242:PHE:N	2.53	0.41
1:D:4034:LYS:HE2	1:D:4034:LYS:HB2	1.84	0.41
1:B:2042:LYS:HE2	1:B:2042:LYS:HB2	1.88	0.41
1:B:2026:ILE:HD13	1:B:2038:VAL:HG23	2.01	0.41
1:D:4178:LEU:N	1:D:4178:LEU:HD23	2.35	0.41
1:D:4164:ASN:HD22	1:D:4164:ASN:HA	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2023:LYS:HD3	1:B:2126:PHE:CZ	2.56	0.41
1:B:2147:MET:HE2	1:B:2147:MET:HB2	1.90	0.41
1:D:4176:ILE:HD11	1:D:4253:VAL:HG13	2.01	0.41
1:C:3213:GLU:HA	1:C:3213:GLU:OE2	2.20	0.41
1:C:3123:VAL:HG21	1:C:3257:LEU:CD1	2.50	0.41
1:B:2022:LYS:NZ	1:B:2260:LEU:HB2	2.36	0.41
1:D:4181:THR:HB	1:D:4183:GLU:OE1	2.21	0.41
1:D:4182:PRO:O	1:D:4186:LEU:N	2.52	0.41
1:D:4181:THR:O	1:D:4184:THR:HB	2.21	0.41
1:C:3039:ASN:HD22	1:C:3042:LYS:HD3	1.86	0.41
1:C:3202:LEU:O	1:C:3202:LEU:HG	2.21	0.40
1:C:3215:TRP:CE2	1:C:3216:LEU:HD21	2.56	0.40
1:D:4170:LEU:HD23	1:D:4170:LEU:HA	1.87	0.40
1:B:2195:ASN:H	1:B:2195:ASN:HD22	1.69	0.40
1:C:3243:LYS:HB3	1:C:3243:LYS:HE2	1.96	0.40
1:B:2195:ASN:N	1:B:2195:ASN:ND2	2.70	0.40
1:D:4120:GLU:HG2	1:D:4121:LYS:HE3	2.01	0.40
1:D:4188:ARG:HA	1:D:4191:LEU:HB2	2.04	0.40
1:A:1086:TYR:CZ	3:A:1401:3L1:H4'	2.56	0.40
1:C:3108:GLN:HB3	1:C:3170:LEU:CD1	2.47	0.40
1:A:1134:ARG:HD3	1:A:1159:HIS:CE1	2.56	0.40
1:D:4240:GLU:OE2	1:D:4245:LYS:HE3	2.20	0.40
1:A:1224:ASN:HA	1:A:1224:ASN:HD22	1.47	0.40
1:A:1053:GLU:O	1:A:1053:GLU:HG3	2.21	0.40
1:B:2175:ILE:HB	1:B:2233:ILE:HG12	2.02	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	215/279 (77%)	187 (87%)	18 (8%)	10 (5%)	<b>3</b> <b>0</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	218/279 (78%)	194 (89%)	22 (10%)	2 (1%)	21	6
1	C	214/279 (77%)	189 (88%)	23 (11%)	2 (1%)	21	6
1	D	211/279 (76%)	190 (90%)	19 (9%)	2 (1%)	21	6
All	All	858/1116 (77%)	760 (89%)	82 (10%)	16 (2%)	10	2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1168	GLN
1	A	1195	ASN
1	B	2114	GLY
1	C	3021	ILE
1	A	1029	ASN
1	A	1193	GLY
1	C	3031	ALA
1	A	1098	THR
1	B	2113	ASN
1	D	4029	ASN
1	A	1112	LEU
1	A	1128	ARG
1	A	1226	ASP
1	D	4102	LEU
1	A	1139	SER
1	A	1209	HIS

### 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	200/255 (78%)	159 (80%)	41 (20%)	1	0
1	B	204/255 (80%)	169 (83%)	35 (17%)	2	0
1	C	199/255 (78%)	158 (79%)	41 (21%)	1	0
1	D	197/255 (77%)	168 (85%)	29 (15%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	800/1020 (78%)	654 (82%)	146 (18%)	<b>2</b> <b>0</b>

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1020	ARG
1	A	1021	ILE
1	A	1023	LYS
1	A	1025	SER
1	A	1038	VAL
1	A	1043	GLN
1	A	1049	GLU
1	A	1050	VAL
1	A	1051	VAL
1	A	1057	ARG
1	A	1087	GLU
1	A	1102	LEU
1	A	1111[A]	SER
1	A	1111[B]	SER
1	A	1112	LEU
1	A	1113	ASN
1	A	1121	LYS
1	A	1132	SER
1	A	1139	SER
1	A	1146	SER
1	A	1163	ASN
1	A	1168	GLN
1	A	1170	LEU
1	A	1171	GLU
1	A	1183	GLU
1	A	1187	HIS
1	A	1189	ILE
1	A	1191	LEU
1	A	1195	ASN
1	A	1200	ILE
1	A	1206	GLU
1	A	1207	LYS
1	A	1219	ARG
1	A	1221	LEU
1	A	1224	ASN
1	A	1226	ASP
1	A	1245	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1251	GLU
1	A	1255	GLU
1	A	1258	SER
1	A	1259	THR
1	B	2038	VAL
1	B	2041	LEU
1	B	2042	LYS
1	B	2060	ASN
1	B	2074	SER
1	B	2075	GLN
1	B	2076	LYS
1	B	2084	MET
1	B	2087	GLU
1	B	2102	LEU
1	B	2105	ILE
1	B	2108	GLN
1	B	2112	LEU
1	B	2115	LYS
1	B	2124	LEU
1	B	2132	SER
1	B	2144	SER
1	B	2147	MET
1	B	2153	THR
1	B	2156	GLN
1	B	2169	SER
1	B	2172	LEU
1	B	2195	ASN
1	B	2198	GLN
1	B	2214	SER
1	B	2217	LEU
1	B	2220	THR
1	B	2222	LYS
1	B	2228	LEU
1	B	2229	GLN
1	B	2235	THR
1	B	2243	LYS
1	B	2248	SER
1	B	2254	LYS
1	B	2259	THR
1	C	3020	ARG
1	C	3023	LYS
1	C	3035	SER

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Mol	Chain	Res	Type
1	C	3046	GLU
1	C	3047	ASP
1	C	3049	GLU
1	C	3051	VAL
1	C	3055	VAL
1	C	3074	SER
1	C	3081	VAL
1	C	3083	GLN
1	C	3093	SER
1	C	3113	ASN
1	C	3122	PRO
1	C	3130	VAL
1	C	3143	GLU
1	C	3147	MET
1	C	3157	ASP
1	C	3162	MET
1	C	3163	ASN
1	C	3165[A]	GLN
1	C	3165[B]	GLN
1	C	3166	PHE
1	C	3170	LEU
1	C	3176	ILE
1	C	3183	GLU
1	C	3186	LEU
1	C	3188	ARG
1	C	3191	LEU
1	C	3195	ASN
1	C	3203	GLU
1	C	3206	GLU
1	C	3207	LYS
1	C	3214	SER
1	C	3219	ARG
1	C	3222	LYS
1	C	3235	THR
1	C	3241	ASP
1	C	3254	LYS
1	C	3258	SER
1	C	3260	LEU
1	D	4020	ARG
1	D	4021	ILE
1	D	4022	LYS
1	D	4039	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	4042	LYS
1	D	4046	GLU
1	D	4081	VAL
1	D	4085	MET
1	D	4086	TYR
1	D	4087[A]	GLU
1	D	4087[B]	GLU
1	D	4104	ARG
1	D	4164	ASN
1	D	4171	GLU
1	D	4191	LEU
1	D	4200	ILE
1	D	4205	LEU
1	D	4214	SER
1	D	4217	LEU
1	D	4219	ARG
1	D	4220	THR
1	D	4221	LEU
1	D	4223	THR
1	D	4227	TYR
1	D	4238	VAL
1	D	4241	ASP
1	D	4245	LYS
1	D	4252	LYS
1	D	4254	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1039	ASN
1	A	1080	ASN
1	A	1083	GLN
1	A	1156	GLN
1	A	1168	GLN
1	A	1195	ASN
1	A	1198	GLN
1	A	1209	HIS
1	A	1224	ASN
1	A	1229	GLN
1	B	2060	ASN
1	B	2075	GLN
1	B	2156	GLN

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Mol	Chain	Res	Type
1	B	2195	ASN
1	B	2229	GLN
1	C	3039	ASN
1	C	3159	HIS
1	C	3163	ASN
1	C	3164	ASN
1	C	3218	HIS
1	D	4039	ASN
1	D	4080	ASN
1	D	4163	ASN
1	D	4164	ASN
1	D	4218	HIS
1	D	4224	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](#)

8 ligands are modelled in this entry.

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	UDP	A	1301	-	18,26,26	1.34	3 (16%)	26,40,40	1.70	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	3L1	A	1401	-	16,20,20	2.17	2 (12%)	17,29,29	4.81	5 (29%)
2	UDP	B	2301	-	18,26,26	1.30	3 (16%)	26,40,40	1.45	3 (11%)
3	3L1	B	2401	-	16,20,20	2.18	3 (18%)	17,29,29	5.00	4 (23%)
2	UDP	C	3301	-	18,26,26	1.31	2 (11%)	26,40,40	1.57	3 (11%)
3	3L1	C	3401	-	16,20,20	2.19	3 (18%)	17,29,29	4.98	5 (29%)
2	UDP	D	4301	-	18,26,26	1.33	3 (16%)	26,40,40	1.38	3 (11%)
3	3L1	D	4401	-	16,20,20	2.21	3 (18%)	17,29,29	4.85	6 (35%)

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	UDP	A	1301	-	-	0/12/32/32	0/2/2/2
3	3L1	A	1401	-	-	0/2/18/18	0/3/3/3
2	UDP	B	2301	-	-	0/12/32/32	0/2/2/2
3	3L1	B	2401	-	-	0/2/18/18	0/3/3/3
2	UDP	C	3301	-	-	0/12/32/32	0/2/2/2
3	3L1	C	3401	-	-	0/2/18/18	0/3/3/3
2	UDP	D	4301	-	-	0/12/32/32	0/2/2/2
3	3L1	D	4401	-	-	0/2/18/18	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	UDP	PB-O3B	-2.62	1.45	1.54
2	C	3301	UDP	PB-O3B	-2.56	1.45	1.54
2	D	4301	UDP	PB-O3B	-2.54	1.45	1.54
2	D	4301	UDP	PA-O2A	-2.29	1.45	1.54
2	B	2301	UDP	PA-O2A	-2.16	1.45	1.54
3	D	4401	3L1	C6-N6	-2.13	1.28	1.34
2	B	2301	UDP	PB-O3B	-2.07	1.47	1.54
3	B	2401	3L1	C6-N6	-2.03	1.28	1.34
3	C	3401	3L1	C6-N6	-2.03	1.28	1.34
2	A	1301	UDP	PA-O2A	-2.03	1.46	1.54
2	A	1301	UDP	C4-N3	2.60	1.37	1.33
2	C	3301	UDP	C4-N3	2.60	1.37	1.33
2	D	4301	UDP	C4-N3	2.69	1.38	1.33
2	B	2301	UDP	C4-N3	2.93	1.38	1.33
3	A	1401	3L1	C2-N1	4.10	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2401	3L1	C2-N1	4.37	1.42	1.33
3	C	3401	3L1	C2-N1	4.47	1.42	1.33
3	D	4401	3L1	C2-N1	4.52	1.42	1.33
3	B	2401	3L1	C2-N3	6.38	1.43	1.32
3	C	3401	3L1	C2-N3	6.40	1.43	1.32
3	D	4401	3L1	C2-N3	6.41	1.43	1.32
3	A	1401	3L1	C2-N3	6.55	1.43	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2401	3L1	N3-C2-N1	-19.32	114.10	128.89
3	C	3401	3L1	N3-C2-N1	-18.99	114.35	128.89
3	D	4401	3L1	N3-C2-N1	-18.33	114.86	128.89
3	A	1401	3L1	N3-C2-N1	-18.09	115.05	128.89
3	A	1401	3L1	C4-C5-N7	-3.25	106.49	109.48
3	B	2401	3L1	C4-C5-N7	-2.55	107.13	109.48
3	A	1401	3L1	O4'-C1'-N9	-2.50	103.39	107.72
3	D	4401	3L1	C4-C5-N7	-2.23	107.43	109.48
2	A	1301	UDP	PA-O3A-PB	-2.22	125.22	132.67
2	A	1301	UDP	O3A-PA-O5'	-2.22	97.06	102.94
3	C	3401	3L1	C4-C5-N7	-2.14	107.51	109.48
3	C	3401	3L1	C1'-N9-C4	2.03	130.60	127.16
3	D	4401	3L1	C1'-N9-C4	2.05	130.62	127.16
2	D	4301	UDP	O5'-PA-O1A	2.21	118.21	109.62
2	C	3301	UDP	O5'-PA-O1A	2.23	118.28	109.62
3	D	4401	3L1	O4'-C1'-C2'	2.27	110.79	106.27
2	A	1301	UDP	O5'-PA-O1A	2.29	118.49	109.62
3	B	2401	3L1	N6-C6-N1	2.45	124.46	119.20
3	A	1401	3L1	N6-C6-N1	2.50	124.57	119.20
3	D	4401	3L1	N6-C6-N1	2.97	125.58	119.20
2	B	2301	UDP	O4'-C1'-N1	3.03	114.46	108.08
3	C	3401	3L1	N6-C6-N1	3.15	125.97	119.20
2	B	2301	UDP	C4-N3-C2	3.21	117.32	114.14
2	D	4301	UDP	O3B-PB-O1B	3.29	121.16	110.58
2	C	3301	UDP	C4-N3-C2	3.59	117.70	114.14
2	D	4301	UDP	C4-N3-C2	3.80	117.91	114.14
2	B	2301	UDP	O3B-PB-O1B	3.88	123.08	110.58
2	A	1301	UDP	O3B-PB-O1B	3.91	123.16	110.58
2	C	3301	UDP	O3B-PB-O1B	4.82	126.09	110.58
3	D	4401	3L1	C2-N1-C6	5.35	128.32	118.77
3	B	2401	3L1	C2-N1-C6	5.56	128.71	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3401	3L1	C2-N1-C6	5.68	128.92	118.77
2	A	1301	UDP	C4-N3-C2	5.72	119.80	114.14
3	A	1401	3L1	C2-N1-C6	5.94	129.37	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	UDP	2	0
3	A	1401	3L1	2	0
2	C	3301	UDP	3	0
3	C	3401	3L1	2	0
2	D	4301	UDP	4	0
3	D	4401	3L1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	219/279 (78%)	1.81	80 (36%) <b>0</b> <b>0</b>	15, 33, 51, 58	0
1	B	223/279 (79%)	1.57	66 (29%) <b>1</b> <b>1</b>	10, 31, 48, 58	0
1	C	219/279 (78%)	1.86	86 (39%) <b>0</b> <b>0</b>	12, 33, 49, 60	0
1	D	218/279 (78%)	1.68	77 (35%) <b>0</b> <b>0</b>	11, 30, 51, 69	0
All	All	879/1116 (78%)	1.73	309 (35%) <b>0</b> <b>0</b>	10, 32, 51, 69	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3199	GLY	6.9
1	A	1166	PHE	6.6
1	B	2114	GLY	6.1
1	A	1168	GLN	5.8
1	C	3221	LEU	5.8
1	B	2221	LEU	5.6
1	D	4190	TYR	5.5
1	C	3112	LEU	5.4
1	A	1195	ASN	5.3
1	C	3166	PHE	5.3
1	B	2195	ASN	5.2
1	A	1191	LEU	5.0
1	B	2228	LEU	5.0
1	D	4158	TRP	4.7
1	B	2199	GLY	4.7
1	A	1210	TYR	4.6
1	C	3200	ILE	4.6
1	A	1193	GLY	4.6
1	C	3020	ARG	4.5
1	A	1204	TYR	4.5
1	D	4210	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	4195	ASN	4.5
1	D	4199	GLY	4.4
1	B	2101	CYS	4.3
1	C	3176	ILE	4.3
1	C	3051	VAL	4.3
1	A	1200	ILE	4.2
1	C	3189	ILE	4.2
1	C	3161	TRP	4.2
1	A	1190	TYR	4.2
1	C	3164	ASN	4.1
1	C	3105	ILE	4.1
1	B	2026	ILE	4.1
1	C	3191	LEU	4.1
1	A	1130	VAL	4.1
1	A	1259	THR	4.0
1	A	1196	GLU	4.0
1	A	1131	TYR	4.0
1	D	4221	LEU	4.0
1	C	3055	VAL	4.0
1	C	3100	ALA	4.0
1	A	1229	GLN	4.0
1	A	1217	LEU	4.0
1	D	4193	GLY	3.9
1	B	2058	TRP	3.9
1	A	1057	ARG	3.9
1	C	3162	MET	3.9
1	A	1169	SER	3.9
1	C	3126	PHE	3.9
1	B	2041	LEU	3.8
1	C	3234	LEU	3.8
1	C	3137	PHE	3.8
1	D	4114	GLY	3.8
1	C	3158	TRP	3.8
1	D	4162	MET	3.8
1	D	4217	LEU	3.7
1	D	4096	PHE	3.7
1	D	4227	TYR	3.7
1	B	2075	GLN	3.7
1	B	2158	TRP	3.7
1	A	1178	LEU	3.7
1	A	1180	ALA	3.7
1	B	2231[A]	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	4222	LYS	3.6
1	C	3098	THR	3.6
1	A	1110	ALA	3.6
1	A	1024	ILE	3.6
1	B	2116	LEU	3.6
1	A	1126	PHE	3.5
1	C	3178	LEU	3.5
1	C	3228	LEU	3.5
1	A	1225	PHE	3.4
1	A	1020	ARG	3.4
1	D	4021	ILE	3.4
1	D	4026	ILE	3.4
1	C	3231	VAL	3.4
1	B	2074	SER	3.4
1	B	2120	GLU	3.4
1	C	3101	CYS	3.4
1	B	2225	PHE	3.4
1	D	4098	THR	3.4
1	B	2130	VAL	3.3
1	D	4244	ASP	3.3
1	B	2229	GLN	3.3
1	B	2187	HIS	3.3
1	D	4203	GLU	3.3
1	C	3260	LEU	3.3
1	A	1094	PHE	3.3
1	A	1096	PHE	3.3
1	A	1101	CYS	3.3
1	C	3181	THR	3.3
1	D	4166	PHE	3.3
1	D	4164	ASN	3.3
1	A	1199	GLY	3.2
1	C	3131	TYR	3.2
1	A	1082	LEU	3.2
1	A	1050	VAL	3.2
1	D	4130	VAL	3.2
1	A	1125	PHE	3.1
1	B	2249	LEU	3.1
1	D	4041	LEU	3.1
1	C	3075	GLN	3.1
1	A	1214	SER	3.1
1	D	4137	PHE	3.1
1	C	3074	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	4176	ILE	3.1
1	D	4038	VAL	3.1
1	C	3124	LEU	3.1
1	C	3073	MET	3.1
1	D	4100	ALA	3.1
1	A	1155	TYR	3.0
1	B	2131	TYR	3.0
1	A	1100	ALA	3.0
1	B	2094	PHE	3.0
1	D	4081	VAL	3.0
1	A	1189	ILE	3.0
1	D	4105	ILE	3.0
1	A	1224	ASN	3.0
1	D	4102	LEU	3.0
1	D	4136	ILE	3.0
1	C	3028	GLY	3.0
1	D	4113	ASN	3.0
1	B	2162	MET	3.0
1	B	2210	TYR	3.0
1	A	1038	VAL	3.0
1	D	4055	VAL	3.0
1	C	3096	PHE	3.0
1	D	4216	LEU	3.0
1	A	1058	TRP	2.9
1	B	2020	ARG	2.9
1	A	1124	LEU	2.9
1	C	3155	TYR	2.9
1	C	3021	ILE	2.9
1	A	1048	TRP	2.9
1	A	1215	TRP	2.9
1	D	4132	SER	2.9
1	B	2095	THR	2.9
1	B	2222	LYS	2.9
1	C	3165[A]	GLN	2.9
1	A	1203	GLU	2.9
1	A	1154	ILE	2.9
1	C	3024	ILE	2.9
1	C	3026	ILE	2.9
1	D	4236	LEU	2.8
1	B	2226	ASP	2.8
1	D	4218	HIS	2.8
1	C	3056	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1095	THR	2.8
1	C	3202	LEU	2.8
1	C	3094	PHE	2.8
1	D	4101	CYS	2.8
1	B	2121	LYS	2.8
1	C	3230	GLU	2.8
1	A	1098	THR	2.8
1	D	4129	SER	2.8
1	A	1055	VAL	2.8
1	C	3030	ILE	2.8
1	C	3136	ILE	2.8
1	D	4177	TYR	2.8
1	B	2123	VAL	2.8
1	B	2177	TYR	2.7
1	D	4200	ILE	2.7
1	A	1157	ASP	2.7
1	D	4235	THR	2.7
1	D	4043	GLN	2.7
1	D	4120	GLU	2.7
1	A	1186	LEU	2.7
1	D	4228	LEU	2.7
1	C	3159	HIS	2.7
1	D	4020	ARG	2.7
1	B	2105	ILE	2.6
1	C	3102	LEU	2.6
1	C	3217	LEU	2.6
1	C	3236	LEU	2.6
1	B	2079	GLY	2.6
1	C	3187	HIS	2.6
1	A	1201	PRO	2.6
1	D	4126	PHE	2.6
1	D	4225	PHE	2.6
1	B	2185	CYS	2.6
1	A	1132	SER	2.6
1	D	4253	VAL	2.6
1	B	2200	ILE	2.6
1	D	4030	ILE	2.6
1	D	4175	ILE	2.6
1	A	1181	THR	2.5
1	B	2111	SER	2.5
1	B	2132	SER	2.5
1	B	2161	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1122	PRO	2.5
1	D	4024	ILE	2.5
1	A	1221	LEU	2.5
1	D	4135	TYR	2.5
1	A	1051	VAL	2.5
1	C	3048	TRP	2.5
1	C	3249	LEU	2.5
1	D	4141	LEU	2.5
1	A	1056	ALA	2.5
1	B	2073	MET	2.5
1	A	1243	LYS	2.5
1	A	1158	TRP	2.5
1	D	4152	TRP	2.5
1	D	4181	THR	2.5
1	A	1233	ILE	2.5
1	C	3132	SER	2.5
1	C	3214	SER	2.5
1	C	3130	VAL	2.5
1	B	2205	LEU	2.5
1	C	3141	LEU	2.5
1	D	4186	LEU	2.5
1	B	2043	GLN	2.5
1	C	3227	TYR	2.4
1	D	4258	SER	2.5
1	C	3038	VAL	2.4
1	C	3121	LYS	2.4
1	A	1167	GLY	2.4
1	C	3109	LEU	2.4
1	D	4116	LEU	2.4
1	D	4233	ILE	2.4
1	B	2060	ASN	2.4
1	C	3246	TYR	2.4
1	C	3078	GLY	2.4
1	D	4033	GLY	2.4
1	D	4131	TYR	2.4
1	D	4050	VAL	2.4
1	A	1119	ALA	2.4
1	C	3218	HIS	2.4
1	A	1172	LEU	2.4
1	B	2102	LEU	2.4
1	C	3129	SER	2.4
1	D	4025	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	4095	THR	2.4
1	A	1052	PRO	2.4
1	B	2224	ASN	2.4
1	C	3203	GLU	2.3
1	C	3154	ILE	2.3
1	C	3138	ALA	2.3
1	D	4034	LYS	2.3
1	A	1176	ILE	2.3
1	C	3037	PHE	2.3
1	D	4198	GLN	2.3
1	D	4170	LEU	2.3
1	D	4260	LEU	2.3
1	B	2122	PRO	2.3
1	B	2098	THR	2.3
1	C	3125	PHE	2.3
1	C	3256	PHE	2.3
1	A	1244	ASP	2.3
1	D	4138	ALA	2.3
1	C	3177	TYR	2.3
1	B	2253	VAL	2.3
1	C	3238	VAL	2.3
1	C	3185	CYS	2.3
1	B	2032	ALA	2.2
1	C	3120	GLU	2.2
1	B	2124	LEU	2.2
1	B	2191	LEU	2.2
1	B	2217	LEU	2.2
1	C	3152	TRP	2.2
1	B	2051[A]	VAL	2.2
1	B	2096	PHE	2.2
1	B	2208	LEU	2.2
1	A	1194	ARG	2.2
1	C	3128	ARG	2.2
1	A	1246	TYR	2.2
1	A	1226	ASP	2.2
1	B	2126	PHE	2.2
1	A	1187	HIS	2.2
1	A	1092	TRP	2.2
1	A	1152	TRP	2.2
1	B	2163	ASN	2.2
1	C	3163	ASN	2.2
1	D	4205	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2030	ILE	2.2
1	A	1036	THR	2.2
1	A	1081	VAL	2.2
1	A	1043	GLN	2.2
1	C	3223	THR	2.1
1	C	3099	TYR	2.1
1	C	3025	SER	2.1
1	D	4133	ASP	2.1
1	C	3208	LEU	2.1
1	A	1026	ILE	2.1
1	A	1175	ILE	2.1
1	D	4259	THR	2.1
1	D	4092	TRP	2.1
1	A	1111[A]	SER	2.1
1	A	1230	GLU	2.1
1	D	4112	LEU	2.1
1	C	3033	GLY	2.1
1	C	3222	LYS	2.1
1	A	1218	HIS	2.1
1	B	2055	VAL	2.1
1	A	1133	ASP	2.1
1	B	2157	ASP	2.1
1	D	4232	PRO	2.1
1	C	3258	SER	2.1
1	D	4178	LEU	2.1
1	B	2028	GLY	2.0
1	B	2198	GLN	2.0
1	D	4256	PHE	2.0
1	B	2260	LEU	2.0
1	B	2152	TRP	2.0
1	B	2176	ILE	2.0
1	C	3157	ASP	2.0
1	A	1165	GLN	2.0
1	B	2227	TYR	2.0
1	C	3204	TYR	2.0
1	B	2137	PHE	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	3L1	C	3401	18/18	0.76	0.19	-0.07	32,37,42,46	0
3	3L1	B	2401	18/18	0.84	0.16	-0.25	29,34,42,42	0
3	3L1	D	4401	18/18	0.81	0.17	-0.41	22,34,40,44	0
2	UDP	C	3301	25/25	0.87	0.15	-0.99	11,35,43,48	0
2	UDP	D	4301	25/25	0.92	0.13	-1.05	22,31,34,42	0
2	UDP	A	1301	25/25	0.90	0.12	-1.09	18,32,35,37	0
3	3L1	A	1401	18/18	0.83	0.16	-1.14	24,31,36,44	0
2	UDP	B	2301	25/25	0.93	0.11	-1.61	17,26,34,41	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.