



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 07:27 AM EDT

PDB ID : 2Z2C
Title : MURA inhibited by unag-cnicin adduct
Authors : Steinbach, A.; Skarzynski, T.; Scheidig, A.J.; Klein, C.D.
Deposited on : unknown
Resolution : 2.05 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

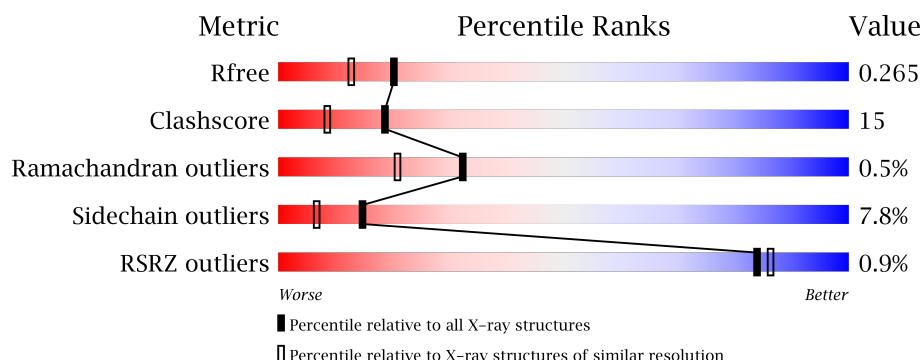
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 72%, yellow 24%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 24% </div> </div>
1	B	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 76%, yellow 19%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 76% 19% </div> </div>
1	C	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 71%, yellow 24%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 71% 24% </div> </div>
1	D	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 67%, yellow 27%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 67% 27% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	IAS	A	67	-	-	X	-
1	IAS	C	67	-	-	X	-
1	IAS	D	67	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13786 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.

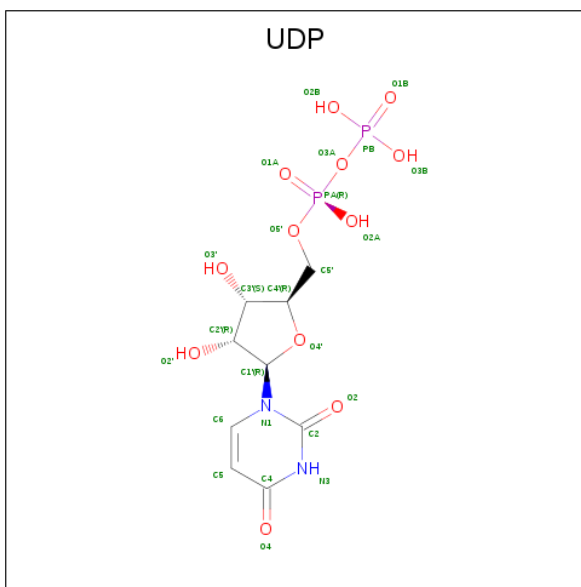
- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	1	0
			3139	1971	558	594	16			
1	B	418	Total	C	N	O	S	0	9	0
			3185	2005	563	601	16			
1	C	418	Total	C	N	O	S	0	3	0
			3153	1982	561	594	16			
1	D	418	Total	C	N	O	S	0	3	0
			3149	1978	559	596	16			

There are 16 discrepancies between the modelled and reference sequences:

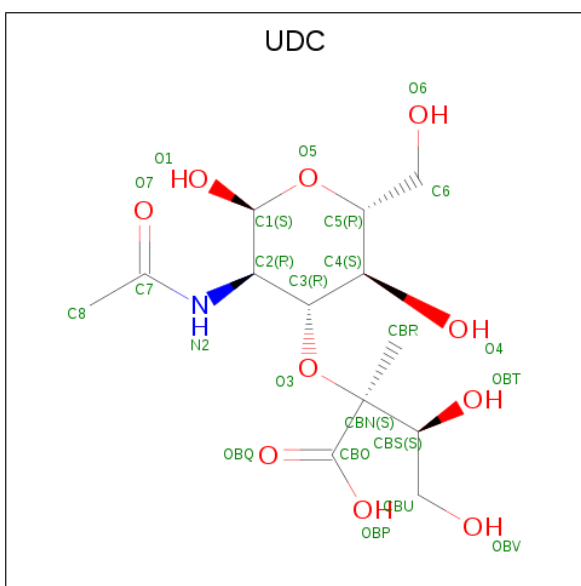
Chain	Residue	Modelled	Actual	Comment	Reference
A	420	LEU	-	SEE REMARK 999	UNP P0A749
A	421	VAL	-	SEE REMARK 999	UNP P0A749
A	422	PRO	-	SEE REMARK 999	UNP P0A749
A	423	ARG	-	SEE REMARK 999	UNP P0A749
B	420	LEU	-	SEE REMARK 999	UNP P0A749
B	421	VAL	-	SEE REMARK 999	UNP P0A749
B	422	PRO	-	SEE REMARK 999	UNP P0A749
B	423	ARG	-	SEE REMARK 999	UNP P0A749
C	420	LEU	-	SEE REMARK 999	UNP P0A749
C	421	VAL	-	SEE REMARK 999	UNP P0A749
C	422	PRO	-	SEE REMARK 999	UNP P0A749
C	423	ARG	-	SEE REMARK 999	UNP P0A749
D	420	LEU	-	SEE REMARK 999	UNP P0A749
D	421	VAL	-	SEE REMARK 999	UNP P0A749
D	422	PRO	-	SEE REMARK 999	UNP P0A749
D	423	ARG	-	SEE REMARK 999	UNP P0A749

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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

- Molecule 3 is 2-(acetylamino)-3-O-[(2S,3S)-2-carboxy-3,4-dihydroxybutan-2-yl]-2-deoxy-alpha-ha-D-glucopyranose (three-letter code: UDC) (formula: C₁₃H₂₃NO₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			32	18	1	13		
3	B	1	Total	C	N	O	0	1
			32	18	1	13		
3	C	1	Total	C	N	O	0	1
			32	18	1	13		
3	D	1	Total	C	N	O	0	1
			32	18	1	13		

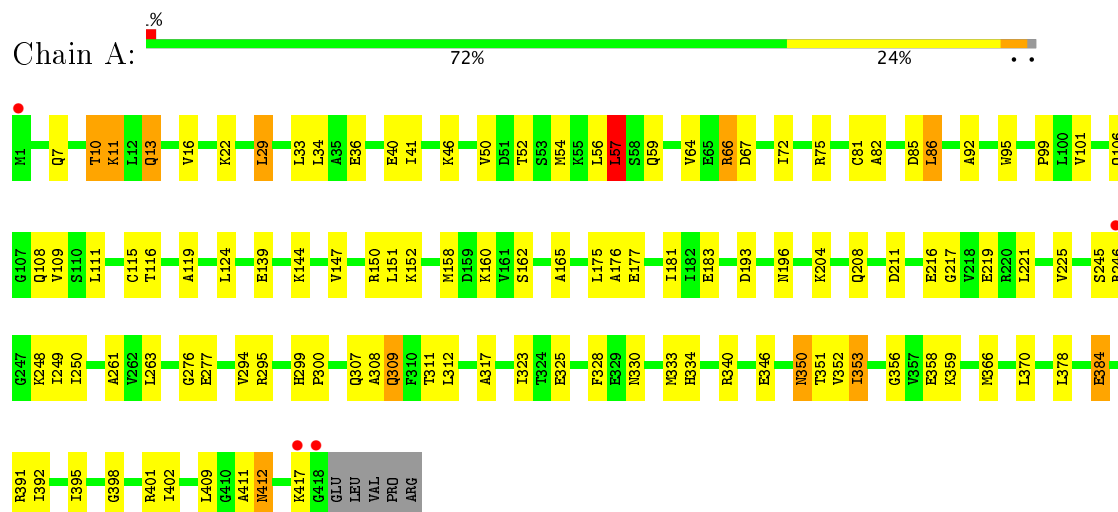
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		
4	B	248	Total	O	0	0
			248	248		
4	C	257	Total	O	0	0
			257	257		
4	D	207	Total	O	0	0
			207	207		

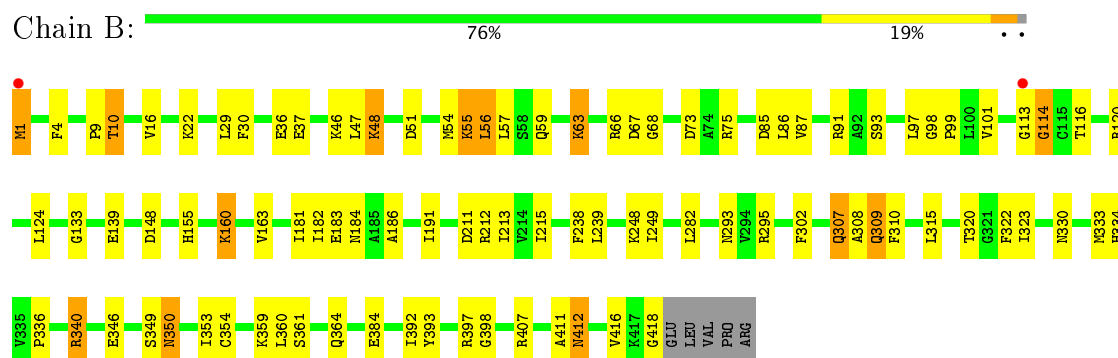
3 Residue-property plots

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

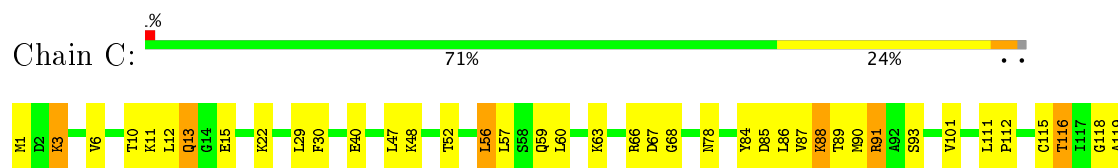
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

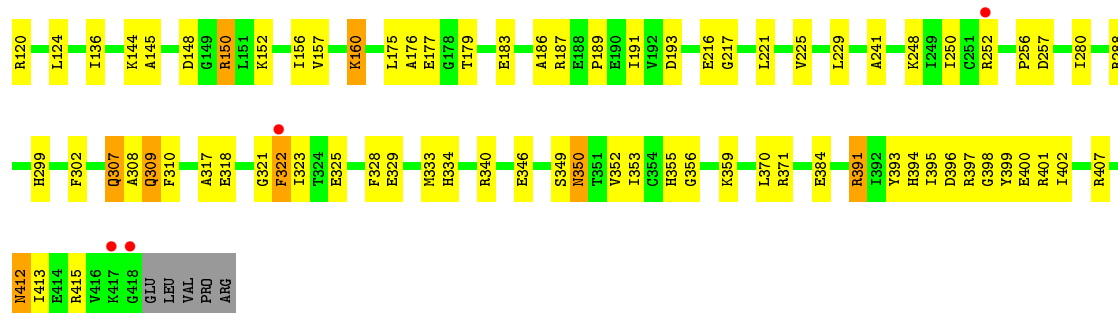


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

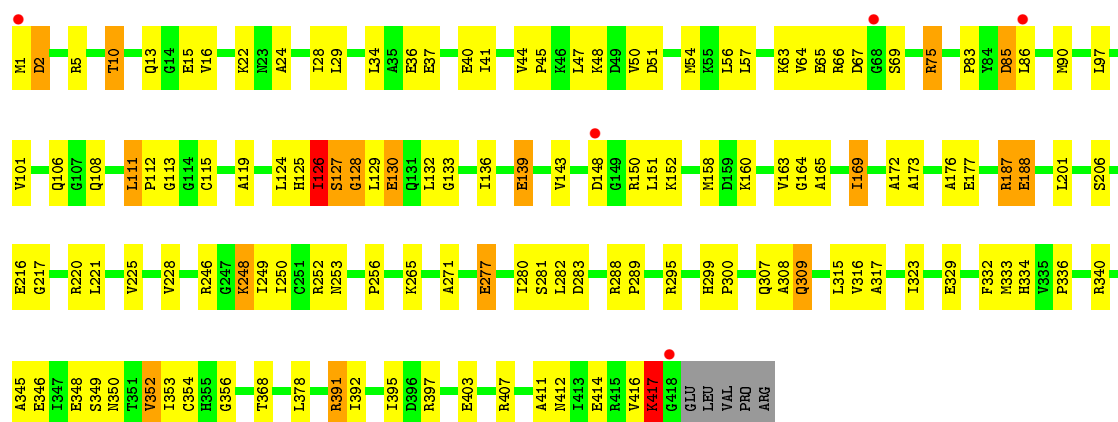


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.13Å 80.37Å 84.87Å 108.69° 111.07° 101.17°	Depositor
Resolution (Å)	19.14 – 2.05 19.14 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.14-2.05) 80.9 (19.14-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.271 0.189 , 0.265	Depositor DCC
R_{free} test set	4202 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13786	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDC, UDP, IAS

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	0.74	0/3179	0.81	1/4304 (0.0%)
1	B	0.77	0/3262	0.83	1/4411 (0.0%)
1	C	0.73	0/3202	0.82	3/4334 (0.1%)
1	D	0.66	0/3197	0.79	1/4327 (0.0%)
All	All	0.73	0/12840	0.81	6/17376 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	C	371	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	D	127	SER	N-CA-C	-6.19	94.30	111.00
1	C	91	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	340	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	57	LEU	CA-CB-CG	5.32	127.53	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	66	ARG	Mainchain
1	D	113	GLY	Peptide
1	D	126	ILE	Peptide

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	3139	0	3214	87	1
1	B	3185	0	3264	91	1
1	C	3153	0	3228	110	0
1	D	3149	0	3225	104	0
2	A	25	0	11	1	0
2	B	25	0	11	0	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
3	A	32	0	15	4	0
3	B	32	0	15	5	0
3	C	32	0	15	9	0
3	D	32	0	16	3	0
4	A	220	0	0	7	0
4	B	248	0	0	17	0
4	C	257	0	0	18	0
4	D	207	0	0	20	0
All	All	13786	0	13036	380	1

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 15.

All (380) 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:C:66:ARG:C	1:C:67:IAS:N	1.74	1.41
1:A:66:ARG:C	1:A:67:IAS:N	1.76	1.38
1:B:350:ASN:HB3	4:B:1012:HOH:O	1.36	1.26
1:D:66:ARG:C	1:D:67:IAS:N	1.94	1.21
1:D:1:MET:HG2	1:D:391:ARG:HH21	1.16	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:HD3	4:B:1201:HOH:O	1.52	1.09
1:C:88:LYS:HE2	1:C:112:PRO:HA	1.35	1.08
1:C:252:ARG:HG2	4:C:1220:HOH:O	1.52	1.08
1:C:120:ARG:NH2	3:C:971[A]:UDC:OBV	1.86	1.07
1:A:66:ARG:C	1:A:67:IAS:H	1.47	1.06
1:D:133:GLY:N	4:D:1063:HOH:O	1.59	1.05
1:C:66:ARG:C	1:C:67:IAS:H	1.46	1.03
1:B:346:GLU:OE1	1:C:322[A]:PHE:CZ	2.12	1.03
1:D:172:ALA:C	4:D:1180:HOH:O	1.96	1.02
1:C:391:ARG:HG2	1:C:391:ARG:HH11	1.22	0.99
1:D:1:MET:HG2	1:D:391:ARG:NH2	1.78	0.98
1:B:309:GLN:H	1:B:309:GLN:HE21	1.13	0.95
1:C:120:ARG:HH22	3:C:971[A]:UDC:HOBV	1.06	0.93
1:C:116:THR:OG1	1:C:333:MET:HE1	1.69	0.93
1:A:309:GLN:HE21	1:A:309:GLN:H	1.07	0.93
1:B:346:GLU:OE1	1:C:322[A]:PHE:HZ	1.50	0.92
1:D:309:GLN:HE21	1:D:309:GLN:H	1.14	0.90
1:D:119:ALA:HB3	4:D:1062:HOH:O	1.70	0.90
1:A:359:LYS:HE3	1:A:384:GLU:HG3	1.51	0.90
1:D:127:SER:C	4:D:1117:HOH:O	2.10	0.89
1:B:359[A]:LYS:HZ2	1:B:384:GLU:HB2	1.39	0.84
1:D:66:ARG:C	1:D:67:IAS:H2	1.80	0.83
1:C:13:GLN:OE1	4:C:1157:HOH:O	1.95	0.83
1:D:165:ALA:O	1:D:169:ILE:HD13	1.82	0.80
1:C:66:ARG:CA	1:C:67:IAS:N	2.44	0.80
1:C:396:ASP:OD2	1:C:415:ARG:NH2	2.14	0.79
1:C:391:ARG:HG2	1:C:391:ARG:NH1	1.90	0.78
1:B:99:PRO:HD3	4:B:1158:HOH:O	1.83	0.78
1:D:128:GLY:N	4:D:1117:HOH:O	2.15	0.78
1:C:87:VAL:HG12	1:C:88:LYS:HE3	1.66	0.78
1:D:130:GLU:N	4:D:1156:HOH:O	2.18	0.77
1:C:67:IAS:OD1	1:C:68:GLY:N	2.17	0.76
1:D:176:ALA:O	1:D:217:GLY:HA3	1.84	0.76
1:B:120:ARG:HH22	3:B:961[A]:UDC:CBU	1.99	0.76
1:B:346:GLU:OE1	1:C:322[A]:PHE:CE2	2.38	0.76
1:D:16:VAL:HG12	1:D:249:ILE:HD11	1.67	0.75
1:A:204:LYS:HD3	1:A:216:GLU:HB3	1.69	0.74
1:D:417:LYS:O	4:D:1153:HOH:O	2.05	0.74
1:D:124:LEU:HD11	1:D:160:LYS:HB2	1.68	0.74
1:C:116:THR:OG1	1:C:333:MET:CE	2.35	0.73
1:C:66:ARG:CA	1:C:67:IAS:H	2.01	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:HG21	1:A:411:ALA:HA	1.70	0.72
1:C:91:ARG:HD3	4:C:1211:HOH:O	1.89	0.72
1:C:120:ARG:HH12	3:C:971[B]:UDC:HBUA	1.54	0.72
1:C:84:TYR:CZ	1:C:88:LYS:HG3	2.26	0.71
1:D:127:SER:O	1:D:130:GLU:HB2	1.90	0.71
4:C:1112:HOH:O	1:D:139:GLU:HG2	1.91	0.70
1:D:173:ALA:N	4:D:1180:HOH:O	2.16	0.69
4:C:1154:HOH:O	1:D:333:MET:HG2	1.91	0.69
1:D:66:ARG:C	1:D:67:IAS:H	1.90	0.69
1:C:84:TYR:CE1	1:C:88:LYS:HG3	2.26	0.69
1:D:126:ILE:HG22	1:D:136:ILE:HD13	1.75	0.69
1:C:359:LYS:HE3	1:C:384:GLU:OE2	1.93	0.69
1:D:130:GLU:O	1:D:132:LEU:O	2.10	0.69
1:A:351:THR:HG21	1:D:348:GLU:HG2	1.74	0.69
1:B:350:ASN:ND2	4:B:1200:HOH:O	2.25	0.69
1:C:59:GLN:HE22	1:C:86:LEU:CD2	2.06	0.69
1:D:248:LYS:HA	1:D:282:LEU:O	1.93	0.68
1:D:316:VAL:O	4:D:1181:HOH:O	2.10	0.68
1:D:64:VAL:O	1:D:65[A]:GLU:HG3	1.94	0.68
1:A:366:MET:HG3	1:A:391:ARG:HD2	1.74	0.68
1:D:115:CYS:SG	4:D:1168:HOH:O	2.27	0.68
1:A:309:GLN:HE21	1:A:309:GLN:N	1.89	0.68
1:A:359:LYS:CE	1:A:384:GLU:HG3	2.23	0.67
1:C:59:GLN:HE22	1:C:86:LEU:HD23	1.59	0.67
1:B:322[B]:PHE:CE1	1:C:353:ILE:HG21	2.29	0.67
1:B:350:ASN:HD22	1:B:350:ASN:H	1.42	0.66
1:D:126:ILE:HG21	1:D:143:VAL:HG11	1.76	0.66
1:B:10:THR:HG21	1:B:411:ALA:HA	1.77	0.66
1:C:150:ARG:CZ	4:C:1080:HOH:O	2.44	0.66
1:C:309:GLN:H	1:C:309:GLN:HE21	1.41	0.66
1:C:412:ASN:C	1:C:412:ASN:HD22	2.00	0.66
1:B:46:LYS:NZ	1:B:67:IAS:OXT	2.29	0.65
1:D:129:LEU:C	4:D:1156:HOH:O	2.33	0.65
1:A:116:THR:HG23	1:A:333:MET:HE1	1.77	0.65
1:B:184:ASN:ND2	4:B:1191:HOH:O	2.28	0.65
1:D:295:ARG:HD3	4:D:987:HOH:O	1.95	0.65
4:A:1078:HOH:O	1:B:333:MET:HG2	1.96	0.65
1:A:359:LYS:HE3	1:A:384:GLU:CG	2.27	0.64
1:A:261:ALA:HA	1:C:157:VAL:HG11	1.79	0.64
1:B:416:VAL:HG12	1:B:418:GLY:H	1.62	0.63
1:B:334:HIS:H	1:B:334:HIS:CD2	2.16	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLN:HA	1:A:13:GLN:OE1	1.99	0.63
1:B:359[B]:LYS:HE2	1:B:384:GLU:HB2	1.79	0.63
1:B:116:THR:HB	1:B:333:MET:CE	2.28	0.63
1:D:34:LEU:HB3	1:D:221:LEU:HD12	1.81	0.63
1:B:124:LEU:HD11	1:B:160:LYS:HG3	1.81	0.62
1:B:322[B]:PHE:CD1	1:C:353:ILE:HD13	2.35	0.62
1:B:186:ALA:HB3	1:B:191:ILE:CD1	2.30	0.62
1:C:40:GLU:HB3	1:C:225:VAL:HG22	1.80	0.62
1:B:91:ARG:HG3	4:B:1120:HOH:O	1.99	0.62
1:C:120:ARG:NH2	3:C:971[A]:UDC:HOBV	1.80	0.62
1:B:359[A]:LYS:NZ	1:B:384:GLU:HB2	2.12	0.61
1:A:366:MET:CG	1:A:391:ARG:HD2	2.31	0.61
1:C:11:LYS:HZ3	1:C:13:GLN:HB3	1.66	0.61
1:A:325:GLU:HG3	1:A:328:PHE:O	1.99	0.61
1:D:334:HIS:H	1:D:334:HIS:CD2	2.18	0.61
1:B:97:LEU:O	1:B:101:VAL:HG23	2.00	0.61
1:D:16:VAL:CG1	1:D:249:ILE:HD11	2.31	0.60
1:C:30:PHE:HE1	1:C:56:LEU:HD12	1.67	0.60
1:B:397:ARG:CZ	4:B:1185:HOH:O	2.49	0.60
1:A:52:THR:HG23	1:A:86:LEU:CD2	2.32	0.60
1:A:22:LYS:HZ1	3:A:951[A]:UDC:HBS	1.66	0.60
1:D:248:LYS:HE2	1:D:250:ILE:HD11	1.84	0.60
1:A:211:ASP:HB3	1:C:187:ARG:HH21	1.66	0.59
1:B:113:GLY:O	1:B:114:GLY:O	2.20	0.59
1:A:412:ASN:HD22	1:A:412:ASN:C	2.05	0.59
1:A:309:GLN:NE2	1:A:309:GLN:H	1.90	0.59
1:D:5:ARG:NH1	1:D:414:GLU:OE1	2.35	0.59
1:C:407:ARG:HD3	4:C:1001:HOH:O	2.02	0.59
1:B:322[B]:PHE:HZ	1:C:355:HIS:CE1	2.21	0.59
1:C:66:ARG:C	1:C:67:IAS:CA	2.69	0.59
1:B:30:PHE:HE1	1:B:56:LEU:HD13	1.68	0.58
1:C:334:HIS:CD2	1:C:334:HIS:H	2.21	0.58
1:D:22:LYS:HB2	1:D:47:LEU:CD1	2.33	0.58
1:B:322[B]:PHE:CE2	1:C:346:GLU:OE1	2.57	0.58
1:C:307:GLN:HG2	1:C:323:ILE:HG21	1.85	0.58
1:A:52:THR:CG2	1:A:86:LEU:HD23	2.34	0.58
1:A:334:HIS:CD2	1:A:334:HIS:H	2.20	0.58
1:C:22:LYS:HD2	1:C:398:GLY:HA2	1.86	0.57
1:A:181:ILE:CD1	4:A:1155:HOH:O	2.52	0.57
1:A:50:VAL:O	1:A:54:MET:HG3	2.04	0.57
1:C:30:PHE:HE1	1:C:56:LEU:CD1	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:GLU:HG2	1:D:220:ARG:HE	1.69	0.57
1:B:359[A]:LYS:HG2	1:B:360:LEU:O	2.04	0.57
1:C:6:VAL:HG13	1:C:413:ILE:HG12	1.87	0.57
1:B:407:ARG:HD3	4:B:1177:HOH:O	2.03	0.57
1:C:87:VAL:CG1	1:C:88:LYS:HE3	2.35	0.56
1:B:353:ILE:N	1:B:353:ILE:HD12	2.20	0.56
1:D:51:ASP:HA	1:D:54:MET:HE2	1.88	0.56
1:C:391:ARG:HG3	1:C:393:TYR:HE1	1.69	0.56
1:C:302:PHE:HZ	1:C:310:PHE:CD1	2.23	0.56
1:A:124:LEU:HB2	2:A:950:UDP:O4	2.06	0.56
1:A:246:ARG:N	4:A:984:HOH:O	2.10	0.56
1:D:22:LYS:NZ	3:D:981[A]:UDC:OBT	2.39	0.56
1:A:52:THR:CG2	1:A:86:LEU:CD2	2.85	0.55
1:C:350:ASN:ND2	4:C:1192:HOH:O	2.39	0.55
1:C:186:ALA:HB3	1:C:191:ILE:CD1	2.36	0.55
1:D:130:GLU:C	1:D:132:LEU:O	2.45	0.55
1:A:59:GLN:HE22	1:A:86:LEU:HD12	1.72	0.55
1:C:150:ARG:HD3	1:C:175:LEU:O	2.07	0.55
1:B:322[B]:PHE:HZ	1:C:355:HIS:HE1	1.53	0.55
1:D:334:HIS:HD2	4:D:1148:HOH:O	1.90	0.55
1:B:238:PHE:HB3	1:B:249:ILE:CD1	2.37	0.54
1:A:350:ASN:HD22	1:A:350:ASN:H	1.55	0.54
1:B:182:ILE:O	1:B:212:ARG:HA	2.06	0.54
1:B:309:GLN:N	1:B:309:GLN:HE21	1.94	0.54
1:C:84:TYR:CE1	1:C:88:LYS:CG	2.91	0.54
1:D:323:ILE:HB	1:D:352:VAL:HG13	1.90	0.54
1:C:391:ARG:CG	1:C:391:ARG:HH11	2.08	0.54
1:A:106:GLN:HE21	1:A:108:GLN:HE22	1.56	0.54
1:D:106:GLN:HE21	1:D:108:GLN:HE22	1.54	0.54
1:A:36:GLU:O	1:A:75:ARG:HG2	2.08	0.54
1:A:317:ALA:O	1:A:356:GLY:HA3	2.07	0.53
1:A:392:ILE:O	1:A:395:ILE:HG22	2.08	0.53
1:A:52:THR:HG23	1:A:86:LEU:HD23	1.89	0.53
1:D:163:VAL:HG22	1:D:188:GLU:CG	2.38	0.53
1:D:66:ARG:O	1:D:67:IAS:N	2.41	0.53
1:B:113:GLY:HA3	4:B:1034:HOH:O	2.08	0.53
1:A:150:ARG:HD3	1:A:175:LEU:O	2.09	0.53
1:A:13:GLN:O	1:A:409:LEU:HA	2.09	0.53
1:C:350:ASN:H	1:C:350:ASN:HD22	1.55	0.53
1:C:288:ARG:HD3	1:C:318:GLU:HG2	1.91	0.52
1:D:151:LEU:O	1:D:177:GLU:HG2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HB3	1:A:221:LEU:HD12	1.91	0.52
1:D:150:ARG:HH12	1:D:177:GLU:HB3	1.73	0.52
1:D:67:IAS:N	1:D:67:IAS:OD1	2.42	0.52
1:D:315:LEU:HD21	1:D:345:ALA:HB2	1.92	0.52
1:A:119:ALA:HB1	1:B:336:PRO:HG3	1.90	0.52
1:C:317:ALA:O	1:C:356:GLY:HA3	2.08	0.52
1:A:13:GLN:OE1	1:A:248:LYS:HG2	2.10	0.52
1:B:51[B]:ASP:OD2	1:B:55:LYS:HE3	2.10	0.52
1:C:22:LYS:HE3	4:C:1222:HOH:O	2.09	0.51
1:C:370:LEU:HD22	4:C:1222:HOH:O	2.10	0.51
1:D:308:ALA:HA	1:D:334:HIS:CE1	2.46	0.51
1:C:288:ARG:CD	1:C:318:GLU:HG2	2.40	0.51
1:C:308:ALA:HA	1:C:334:HIS:CE1	2.46	0.51
1:C:152:LYS:HA	1:C:177:GLU:HG3	1.93	0.51
1:D:299:HIS:CG	1:D:300:PRO:HA	2.46	0.51
1:A:66:ARG:C	1:A:67:IAS:CA	2.72	0.51
1:A:162:SER:HB3	1:A:165:ALA:HB3	1.93	0.50
1:C:179:THR:OG1	1:C:216:GLU:OE2	2.21	0.50
1:A:139:GLU:HB2	1:A:144:LYS:HE3	1.93	0.50
1:B:133:GLY:HA3	4:B:1025:HOH:O	2.11	0.50
1:B:9:PRO:HD3	1:B:384:GLU:OE1	2.10	0.50
1:C:48:LYS:HG3	4:C:1050:HOH:O	2.12	0.50
1:C:22:LYS:NZ	3:C:971[A]:UDC:OBP	2.44	0.50
1:D:248:LYS:HD2	1:D:283:ASP:HB2	1.94	0.50
1:C:397:ARG:HD2	4:C:1196:HOH:O	2.11	0.50
1:D:277:GLU:OE2	4:D:1102:HOH:O	2.20	0.50
1:C:15:GLU:HG3	1:C:250:ILE:HB	1.93	0.50
1:B:412:ASN:C	1:B:412:ASN:HD22	2.15	0.50
1:D:85:ASP:N	1:D:85:ASP:OD1	2.41	0.50
1:B:315:LEU:HD23	1:B:354:CYS:HB3	1.94	0.49
1:C:120:ARG:HH12	3:C:971[B]:UDC:CBU	2.23	0.49
1:C:395:ILE:HD11	1:C:402:ILE:HD13	1.95	0.49
1:C:85:ASP:O	1:C:89:THR:HG23	2.12	0.49
1:A:346:GLU:O	1:A:353:ILE:HG12	2.12	0.49
1:B:295:ARG:NE	1:D:160:LYS:HE2	2.28	0.49
1:B:308:ALA:HA	1:B:334:HIS:CE1	2.47	0.49
1:D:111:LEU:HD23	1:D:112:PRO:HD2	1.93	0.49
1:D:83:PRO:HG2	1:D:86:LEU:HD12	1.94	0.48
1:A:150:ARG:HB2	4:A:969:HOH:O	2.12	0.48
1:A:175:LEU:HD21	1:A:221:LEU:HG	1.94	0.48
1:A:350:ASN:N	1:A:350:ASN:HD22	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:PHE:HE2	1:D:350:ASN:HA	1.77	0.48
1:D:54:MET:HE1	1:D:66:ARG:HD2	1.95	0.48
1:A:204:LYS:HB2	1:A:216:GLU:HB3	1.96	0.48
1:A:295:ARG:HD2	1:C:160:LYS:HB3	1.95	0.48
1:B:120:ARG:HH22	3:B:961[A]:UDC:HBU	1.73	0.48
1:C:257:ASP:HB2	4:C:1155:HOH:O	2.13	0.48
1:D:248:LYS:HE2	1:D:250:ILE:CD1	2.42	0.48
1:C:52:THR:HG21	1:C:90:MET:HG2	1.96	0.48
1:B:322[B]:PHE:CZ	1:C:353:ILE:HG21	2.49	0.48
1:B:293:ASN:ND2	1:B:322[B]:PHE:CD2	2.82	0.47
1:C:115:CYS:HB3	1:C:118:GLY:O	2.13	0.47
1:C:101:VAL:CG2	1:C:145:ALA:HB3	2.44	0.47
1:C:394:HIS:HE1	4:C:1007:HOH:O	1.96	0.47
1:C:56:LEU:O	1:C:60:LEU:HG	2.15	0.47
1:D:97:LEU:O	1:D:101:VAL:HG23	2.14	0.47
1:C:13:GLN:NE2	1:C:248:LYS:HB3	2.30	0.47
1:D:24:ALA:HB3	1:D:228:VAL:HG13	1.97	0.47
1:B:120:ARG:NH2	3:B:961[A]:UDC:OBV	2.40	0.47
1:B:98:GLY:HA3	4:B:1158:HOH:O	2.15	0.47
1:C:11:LYS:HZ3	1:C:13:GLN:CB	2.27	0.47
1:D:416:VAL:HG12	1:D:417:LYS:N	2.30	0.47
1:A:33:LEU:HD21	1:A:57:LEU:HD12	1.97	0.46
1:C:309:GLN:N	1:C:309:GLN:HE21	2.11	0.46
1:C:30:PHE:CE1	1:C:56:LEU:HD12	2.49	0.46
1:B:211:ASP:HB3	1:D:187:ARG:HH12	1.80	0.46
1:C:321:GLY:C	1:C:322[A]:PHE:CD1	2.89	0.46
1:D:353:ILE:HD12	1:D:353:ILE:N	2.29	0.46
1:A:263:LEU:HD12	4:A:1098:HOH:O	2.16	0.46
1:B:1:MET:H1	1:B:393:TYR:HD2	1.64	0.46
1:D:40:GLU:HB3	1:D:225:VAL:HG22	1.97	0.46
1:B:239:LEU:HD22	1:B:282:LEU:HB2	1.98	0.46
1:A:330:ASN:HB2	1:B:330:ASN:OD1	2.16	0.46
1:C:397:ARG:NH1	4:C:1222:HOH:O	2.48	0.46
1:D:28:ILE:CG2	1:D:41:ILE:HG12	2.46	0.46
1:A:309:GLN:O	1:A:312:LEU:HB3	2.16	0.46
1:A:52:THR:HG23	1:A:86:LEU:HD21	1.97	0.46
4:C:1215:HOH:O	1:D:119:ALA:HB2	2.16	0.46
1:C:119:ALA:N	1:C:329:GLU:OE2	2.43	0.45
1:A:370:LEU:HD21	1:A:398:GLY:HA3	1.98	0.45
1:D:250:ILE:HG13	1:D:281:SER:HB2	1.98	0.45
1:D:317:ALA:O	1:D:356:GLY:HA3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63[C]:LYS:HB2	1:B:73:ASP:HB3	1.97	0.45
1:D:246:ARG:NH2	1:D:288:ARG:HD2	2.31	0.45
1:D:56:LEU:HD23	1:D:56:LEU:O	2.16	0.45
1:B:302:PHE:HZ	1:B:310:PHE:CD1	2.35	0.45
1:B:59:GLN:HB3	4:B:1075:HOH:O	2.15	0.45
1:A:249:ILE:HG12	1:A:250:ILE:H	1.80	0.45
1:B:155:HIS:CD2	1:B:181:ILE:HB	2.52	0.45
1:A:115:CYS:O	1:A:116:THR:C	2.55	0.45
1:A:334:HIS:HD2	4:A:980:HOH:O	2.00	0.45
1:C:124:LEU:HD11	1:C:160:LYS:HG3	1.99	0.45
1:C:323:ILE:HB	1:C:352:VAL:CG1	2.47	0.45
1:D:403:GLU:O	1:D:407:ARG:HB2	2.17	0.44
1:A:219:GLU:HG2	1:A:219:GLU:O	2.17	0.44
1:A:276:GLY:O	1:A:277:GLU:C	2.55	0.44
1:C:22:LYS:HB2	1:C:47:LEU:CD1	2.47	0.44
1:A:294:VAL:HB	1:A:323:ILE:HD13	1.98	0.44
1:A:11:LYS:HE2	1:A:11:LYS:HB2	1.70	0.44
1:B:47:LEU:HD13	1:B:398:GLY:HA2	1.99	0.44
1:B:51[B]:ASP:OD1	4:B:1020:HOH:O	2.21	0.44
1:D:132:LEU:HD23	1:D:152:LYS:O	2.18	0.44
1:A:340:ARG:CZ	1:A:340:ARG:HB3	2.48	0.44
1:D:392:ILE:O	1:D:395:ILE:HG22	2.18	0.44
1:D:416:VAL:CG1	1:D:417:LYS:N	2.81	0.44
1:A:29:LEU:HD12	1:A:41:ILE:HD13	1.99	0.44
1:A:299:HIS:CG	1:A:300:PRO:HA	2.53	0.44
1:C:176:ALA:O	1:C:217:GLY:HA3	2.17	0.44
1:A:16:VAL:HG12	1:A:249:ILE:HD11	1.99	0.43
1:B:148:ASP:OD1	1:B:148:ASP:C	2.56	0.43
1:B:22:LYS:NZ	3:B:961[B]:UDC:OBT	2.51	0.43
1:C:175:LEU:HD21	1:C:221:LEU:HG	2.00	0.43
1:D:340:ARG:HB3	1:D:340:ARG:CZ	2.48	0.43
1:A:46:LYS:NZ	1:A:67:IAS:O	2.51	0.43
1:A:81:CYS:HA	1:A:108:GLN:O	2.18	0.43
1:A:249:ILE:HG12	1:A:250:ILE:N	2.33	0.43
1:A:92:ALA:O	1:A:95:TRP:HB2	2.18	0.43
1:B:353:ILE:HG21	1:C:322[A]:PHE:CZ	2.53	0.43
1:D:256:PRO:HG3	1:D:280:ILE:HG13	1.98	0.43
1:C:116:THR:HG1	1:C:333:MET:CE	2.28	0.43
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.49	0.43
1:A:211:ASP:HB3	1:C:187:ARG:NH2	2.33	0.43
1:C:399:TYR:HB3	1:C:402:ILE:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LYS:HB3	1:B:397:ARG:HA	1.99	0.43
1:D:288:ARG:HG3	1:D:289:PRO:HD2	2.00	0.43
1:D:119:ALA:N	1:D:329:GLU:OE2	2.43	0.43
1:A:401:ARG:NE	4:A:1033:HOH:O	2.30	0.43
1:B:309:GLN:H	1:B:309:GLN:NE2	1.96	0.43
1:D:13:GLN:HA	1:D:248:LYS:O	2.18	0.43
1:B:68:GLY:N	4:B:1155:HOH:O	2.51	0.43
1:C:333:MET:HG2	4:D:1176:HOH:O	2.18	0.43
1:A:152:LYS:HG2	1:A:177:GLU:HG2	2.01	0.43
1:C:3:LYS:HE3	1:C:3:LYS:HB3	1.64	0.43
1:C:48:LYS:HB3	1:C:397:ARG:HA	2.01	0.43
1:D:22:LYS:HB2	1:D:47:LEU:HD11	2.01	0.43
1:D:64:VAL:C	1:D:65[A]:GLU:HG3	2.39	0.43
1:A:40:GLU:HB3	1:A:225:VAL:HG22	2.00	0.42
1:A:176:ALA:O	1:A:217:GLY:HA3	2.19	0.42
1:A:116:THR:HG23	1:A:333:MET:CE	2.46	0.42
1:A:350:ASN:ND2	1:A:350:ASN:H	2.17	0.42
1:B:87:VAL:HG22	1:B:93:SER:OG	2.20	0.42
1:C:340:ARG:NH1	1:D:111:LEU:O	2.47	0.42
1:B:113:GLY:CA	4:B:1034:HOH:O	2.64	0.42
1:B:163:VAL:HA	1:B:191:ILE:HD11	2.01	0.42
1:B:364:GLN:NE2	4:B:1022:HOH:O	2.52	0.42
1:B:46:LYS:O	1:B:47:LEU:HD23	2.18	0.42
1:D:201:LEU:HB3	1:D:221:LEU:HB3	2.01	0.42
1:B:116:THR:HB	1:B:333:MET:HE2	2.00	0.42
1:B:36:GLU:O	1:B:75:ARG:HG2	2.20	0.42
1:C:12:LEU:CD1	1:C:241:ALA:HB1	2.50	0.42
1:D:50:VAL:O	1:D:54:MET:HG3	2.20	0.42
1:D:22:LYS:HZ1	3:D:981[B]:UDC:HBS	1.83	0.42
1:C:189:PRO:HD3	1:C:299:HIS:CD2	2.55	0.42
1:D:271:ALA:HB1	1:D:282:LEU:HG	2.02	0.42
1:A:308:ALA:HA	1:A:334:HIS:CE1	2.55	0.42
1:B:320:THR:HG22	1:B:322[B]:PHE:CE1	2.55	0.42
1:D:309:GLN:HE21	1:D:309:GLN:N	1.96	0.42
1:D:397:ARG:HD2	4:D:1120:HOH:O	2.20	0.42
1:B:213:ILE:HG22	1:B:215:ILE:CD1	2.51	0.41
1:C:256:PRO:HG3	1:C:280:ILE:HG12	2.02	0.41
1:D:252:ARG:NH2	4:D:1106:HOH:O	2.47	0.41
1:A:181:ILE:N	1:A:181:ILE:HD12	2.35	0.41
1:A:34:LEU:CB	1:A:221:LEU:HD12	2.51	0.41
1:A:64:VAL:HG13	1:A:72:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:CZ	1:B:340:ARG:HB3	2.51	0.41
1:D:125:HIS:CE1	1:D:164:GLY:C	2.93	0.41
1:B:4:PHE:CD2	1:B:392:ILE:HG12	2.56	0.41
1:C:391:ARG:NH1	4:C:1007:HOH:O	2.52	0.41
1:C:412:ASN:C	1:C:412:ASN:ND2	2.72	0.41
1:D:315:LEU:HD23	1:D:354:CYS:HB3	2.01	0.41
1:A:196:ASN:OD1	1:A:208:GLN:NE2	2.53	0.41
3:B:961[A]:UDC:HBU	3:B:961[A]:UDC:HBRA	1.76	0.41
1:C:325:GLU:HG3	1:C:328:PHE:O	2.20	0.41
1:B:22:LYS:HD3	1:B:398:GLY:HA2	2.02	0.41
1:B:307:GLN:HG2	1:B:323:ILE:HG21	2.03	0.41
1:B:139:GLU:HB2	4:B:1198:HOH:O	2.19	0.41
1:D:130:GLU:HG2	4:D:1034:HOH:O	2.20	0.41
1:A:82:ALA:HB3	1:A:109:VAL:HG13	2.03	0.41
1:A:245:SER:O	1:A:246:ARG:HB2	2.21	0.41
1:C:11:LYS:NZ	1:C:13:GLN:CB	2.83	0.41
1:D:173:ALA:CA	4:D:1180:HOH:O	2.65	0.41
1:D:36:GLU:CG	1:D:220:ARG:HE	2.34	0.41
1:C:401:ARG:NH1	4:C:1091:HOH:O	2.48	0.41
1:D:45:PRO:HG2	1:D:47:LEU:CD1	2.51	0.41
1:D:333:MET:HB3	1:D:368:THR:HG21	2.03	0.41
1:D:36:GLU:O	1:D:75:ARG:HG2	2.20	0.41
1:A:147:VAL:HG21	1:A:151:LEU:CD2	2.52	0.40
1:B:55:LYS:HB3	1:B:86:LEU:HD11	2.03	0.40
1:A:95:TRP:O	1:A:99:PRO:HD2	2.21	0.40
1:B:16:VAL:CG1	1:B:249:ILE:HD11	2.51	0.40
1:C:136:ILE:HA	1:C:144:LYS:O	2.20	0.40
1:B:213:ILE:HG22	1:B:215:ILE:HD11	2.02	0.40
1:C:323:ILE:HB	1:C:352:VAL:HG12	2.03	0.40
1:D:349:SER:N	4:D:1178:HOH:O	2.43	0.40
1:A:311:THR:HG21	1:A:334:HIS:CE1	2.56	0.40
1:B:320:THR:HG22	1:B:322[B]:PHE:CZ	2.57	0.40
1:D:10:THR:HG21	1:D:411:ALA:HA	2.04	0.40
1:D:333:MET:O	1:D:336:PRO:HD2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLU:OE2	1:B:10:THR:OG1[1_455]	2.01	0.19

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	415/423 (98%)	398 (96%)	16 (4%)	1 (0%)	51	42
1	B	424/423 (100%)	418 (99%)	4 (1%)	2 (0%)	32	21
1	C	417/423 (99%)	410 (98%)	6 (1%)	1 (0%)	51	42
1	D	417/423 (99%)	400 (96%)	13 (3%)	4 (1%)	18	8
All	All	1673/1692 (99%)	1626 (97%)	39 (2%)	8 (0%)	32	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	GLY
1	D	2	ASP
1	D	128	GLY
1	A	417	LYS
1	B	349	SER
1	C	93	SER
1	D	130	GLU
1	D	417	LYS

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	331/335 (99%)	306 (92%)	25 (8%)	15	7
1	B	340/335 (102%)	321 (94%)	19 (6%)	25	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	333/335 (99%)	305 (92%)	28 (8%)	13 5
1	D	333/335 (99%)	299 (90%)	34 (10%)	8 3
All	All	1337/1340 (100%)	1231 (92%)	106 (8%)	15 6

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	10	THR
1	A	11	LYS
1	A	13	GLN
1	A	29	LEU
1	A	56	LEU
1	A	57	LEU
1	A	66	ARG
1	A	85	ASP
1	A	86	LEU
1	A	101	VAL
1	A	111	LEU
1	A	158	MET
1	A	160	LYS
1	A	183	GLU
1	A	193	ASP
1	A	307	GLN
1	A	309	GLN
1	A	350	ASN
1	A	352	VAL
1	A	353	ILE
1	A	378	LEU
1	A	384	GLU
1	A	402	ILE
1	A	412	ASN
1	B	1	MET
1	B	10	THR
1	B	29	LEU
1	B	37	GLU
1	B	48	LYS
1	B	55	LYS
1	B	56	LEU
1	B	57	LEU
1	B	63[A]	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	63[B]	LYS
1	B	63[C]	LYS
1	B	85	ASP
1	B	160	LYS
1	B	183	GLU
1	B	307	GLN
1	B	309	GLN
1	B	350	ASN
1	B	361	SER
1	B	412	ASN
1	C	1	MET
1	C	3	LYS
1	C	10	THR
1	C	13	GLN
1	C	29	LEU
1	C	56	LEU
1	C	57	LEU
1	C	63	LYS
1	C	78	ASN
1	C	88	LYS
1	C	111	LEU
1	C	116	THR
1	C	148	ASP
1	C	150	ARG
1	C	156	ILE
1	C	160	LYS
1	C	183	GLU
1	C	193	ASP
1	C	229	LEU
1	C	307	GLN
1	C	309	GLN
1	C	322[A]	PHE
1	C	322[B]	PHE
1	C	349	SER
1	C	350	ASN
1	C	391	ARG
1	C	400	GLU
1	C	412	ASN
1	D	2	ASP
1	D	10	THR
1	D	15	GLU
1	D	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	37	GLU
1	D	48	LYS
1	D	57	LEU
1	D	63	LYS
1	D	69	SER
1	D	75	ARG
1	D	85	ASP
1	D	90	MET
1	D	111	LEU
1	D	126	ILE
1	D	139	GLU
1	D	148	ASP
1	D	158	MET
1	D	169	ILE
1	D	187	ARG
1	D	188	GLU
1	D	206	SER
1	D	216	GLU
1	D	248	LYS
1	D	253	ASN
1	D	265	LYS
1	D	277	GLU
1	D	307	GLN
1	D	309	GLN
1	D	346	GLU
1	D	352	VAL
1	D	378	LEU
1	D	391	ARG
1	D	412	ASN
1	D	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	42	GLN
1	A	106	GLN
1	A	184	ASN
1	A	253	ASN
1	A	293	ASN
1	A	309	GLN
1	A	330	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	334	HIS
1	A	350	ASN
1	A	412	ASN
1	B	42	GLN
1	B	155	HIS
1	B	184	ASN
1	B	253	ASN
1	B	293	ASN
1	B	309	GLN
1	B	334	HIS
1	B	350	ASN
1	B	364	GLN
1	B	412	ASN
1	C	13	GLN
1	C	59	GLN
1	C	78	ASN
1	C	131	GLN
1	C	184	ASN
1	C	253	ASN
1	C	293	ASN
1	C	309	GLN
1	C	334	HIS
1	C	350	ASN
1	C	394	HIS
1	C	412	ASN
1	D	42	GLN
1	D	106	GLN
1	D	184	ASN
1	D	253	ASN
1	D	293	ASN
1	D	309	GLN
1	D	334	HIS
1	D	364	GLN
1	D	412	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	IAS	A	67	1	3,7,8	0.96	0	2,8,10	1.12	0
1	IAS	B	67	1	3,7,8	0.84	0	2,8,10	1.61	1 (50%)
1	IAS	C	67	1	3,7,8	0.51	0	2,8,10	0.09	0
1	IAS	D	67	1	3,7,8	0.50	0	2,8,10	1.30	0

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
1	IAS	A	67	1	-	0/3/7/8	0/0/0/0
1	IAS	B	67	1	-	0/3/7/8	0/0/0/0
1	IAS	C	67	1	-	0/3/7/8	0/0/0/0
1	IAS	D	67	1	-	0/3/7/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	IAS	CB-CA-N	-2.28	103.58	112.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	67	IAS	4	0
1	B	67	IAS	1	0
1	C	67	IAS	6	0
1	D	67	IAS	5	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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	950	3	21,26,26	2.27	7 (33%)	22,40,40	2.18	6 (27%)
3	UDC	A	951[A]	-	18,23,24	1.85	4 (22%)	19,33,35	1.56	2 (10%)
3	UDC	A	951[B]	-	18,23,24	1.22	2 (11%)	19,33,35	1.06	1 (5%)
2	UDP	B	960	3	21,26,26	1.94	6 (28%)	22,40,40	1.83	3 (13%)
3	UDC	B	961[A]	-	18,23,24	1.89	3 (16%)	19,33,35	1.41	3 (15%)
3	UDC	B	961[B]	-	18,23,24	1.25	1 (5%)	19,33,35	1.23	2 (10%)
2	UDP	C	970	3	21,26,26	2.17	6 (28%)	22,40,40	1.74	3 (13%)
3	UDC	C	971[A]	-	18,23,24	1.57	3 (16%)	19,33,35	2.02	3 (15%)
3	UDC	C	971[B]	-	18,23,24	1.07	1 (5%)	19,33,35	1.51	2 (10%)
2	UDP	D	980	3	21,26,26	1.84	4 (19%)	22,40,40	2.03	3 (13%)
3	UDC	D	981[A]	-	18,23,24	1.91	6 (33%)	19,33,35	1.77	5 (26%)
3	UDC	D	981[B]	-	18,23,24	1.55	4 (22%)	19,33,35	1.65	4 (21%)

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	950	3	-	0/12/32/32	0/2/2/2
3	UDC	A	951[A]	-	-	0/17/42/45	0/1/1/1
3	UDC	A	951[B]	-	-	0/17/42/45	0/1/1/1
2	UDP	B	960	3	-	0/12/32/32	0/2/2/2
3	UDC	B	961[A]	-	-	0/17/42/45	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDC	B	961[B]	-	-	0/17/42/45	0/1/1/1
2	UDP	C	970	3	-	0/12/32/32	0/2/2/2
3	UDC	C	971[A]	-	-	0/17/42/45	0/1/1/1
3	UDC	C	971[B]	-	-	0/17/42/45	0/1/1/1
2	UDP	D	980	3	-	0/12/32/32	0/2/2/2
3	UDC	D	981[A]	-	-	0/17/42/45	0/1/1/1
3	UDC	D	981[B]	-	-	0/17/42/45	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	951[A]	UDC	OBT-CBS	-5.21	1.34	1.43
3	B	961[A]	UDC	OBT-CBS	-5.01	1.35	1.43
3	C	971[A]	UDC	OBT-CBS	-4.31	1.36	1.43
3	D	981[A]	UDC	OBT-CBS	-3.86	1.37	1.43
3	B	961[A]	UDC	CBU-CBS	-3.27	1.47	1.51
3	D	981[A]	UDC	CBU-CBS	-3.17	1.47	1.51
3	A	951[A]	UDC	CBU-CBS	-3.10	1.47	1.51
2	B	960	UDP	O4'-C1'	-2.77	1.37	1.41
3	C	971[A]	UDC	CBU-CBS	-2.36	1.48	1.51
2	C	970	UDP	PA-O5'	-2.35	1.49	1.59
2	C	970	UDP	PB-O3B	-2.32	1.45	1.54
3	D	981[B]	UDC	O5-C5	-2.31	1.38	1.43
3	D	981[A]	UDC	O5-C5	-2.31	1.38	1.43
2	B	960	UDP	PB-O3B	-2.28	1.45	1.54
2	A	950	UDP	PB-O2B	-2.23	1.45	1.54
3	D	981[B]	UDC	C2-N2	2.05	1.49	1.46
3	D	981[A]	UDC	C2-N2	2.05	1.49	1.46
2	A	950	UDP	C5'-C4'	2.21	1.58	1.51
3	D	981[B]	UDC	C8-C7	2.27	1.55	1.50
3	D	981[A]	UDC	C8-C7	2.27	1.55	1.50
3	C	971[B]	UDC	C6-C5	2.35	1.59	1.51
3	C	971[A]	UDC	C6-C5	2.35	1.59	1.51
3	A	951[B]	UDC	C2-N2	2.36	1.50	1.46
3	A	951[A]	UDC	C2-N2	2.36	1.50	1.46
2	B	960	UDP	PB-O3A	2.43	1.64	1.60
3	A	951[B]	UDC	O5-C1	2.57	1.47	1.43
3	A	951[A]	UDC	O5-C1	2.57	1.47	1.43
2	A	950	UDP	PB-O3A	2.84	1.64	1.60
2	D	980	UDP	PB-O1B	2.93	1.60	1.50
2	C	970	UDP	PB-O1B	2.93	1.60	1.50
2	A	950	UDP	PB-O1B	3.06	1.61	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	960	UDP	PB-O1B	3.13	1.61	1.50
3	B	961[B]	UDC	O3-C3	3.26	1.45	1.42
3	B	961[A]	UDC	O3-C3	3.26	1.45	1.42
2	D	980	UDP	O4'-C1'	3.44	1.46	1.41
2	D	980	UDP	C4-N3	3.44	1.39	1.33
2	A	950	UDP	C4-N3	3.90	1.40	1.33
3	D	981[B]	UDC	O3-C3	4.06	1.46	1.42
3	D	981[A]	UDC	O3-C3	4.06	1.46	1.42
2	A	950	UDP	C6-N1	4.18	1.41	1.35
2	C	970	UDP	C4-N3	4.26	1.40	1.33
2	C	970	UDP	C6-N1	4.30	1.41	1.35
2	B	960	UDP	C6-N1	4.36	1.41	1.35
2	B	960	UDP	C4-N3	4.64	1.41	1.33
2	D	980	UDP	C6-N1	4.66	1.42	1.35
2	C	970	UDP	O4'-C1'	4.84	1.47	1.41
2	A	950	UDP	O4'-C1'	4.84	1.48	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	971[A]	UDC	OBT-CBS-CBU	-5.74	97.88	108.96
3	A	951[A]	UDC	OBT-CBS-CBU	-4.67	99.95	108.96
2	A	950	UDP	O4'-C1'-N1	-3.75	100.57	108.08
3	D	981[B]	UDC	C4-C3-C2	-3.41	105.24	111.18
3	D	981[A]	UDC	C4-C3-C2	-3.41	105.24	111.18
3	D	981[A]	UDC	OBT-CBS-CBU	-3.33	102.54	108.96
3	B	961[A]	UDC	OBT-CBS-CBU	-3.19	102.81	108.96
3	B	961[B]	UDC	O5-C1-C2	-2.98	107.33	111.47
3	B	961[A]	UDC	O5-C1-C2	-2.98	107.33	111.47
2	A	950	UDP	O3A-PB-O1B	-2.57	95.61	111.44
2	A	950	UDP	C4'-O4'-C1'	-2.56	107.04	109.77
2	A	950	UDP	O2'-C2'-C1'	-2.44	103.99	111.61
3	B	961[B]	UDC	C4-C3-C2	-2.29	107.19	111.18
3	B	961[A]	UDC	C4-C3-C2	-2.29	107.19	111.18
2	C	970	UDP	O3A-PB-O1B	-2.29	97.35	111.44
3	D	981[B]	UDC	O3-C3-C2	-2.23	102.46	107.68
3	D	981[A]	UDC	O3-C3-C2	-2.23	102.46	107.68
2	B	960	UDP	O3A-PB-O1B	-2.18	98.04	111.44
3	C	971[B]	UDC	O4-C4-C5	-2.09	104.03	109.28
3	C	971[A]	UDC	O4-C4-C5	-2.09	104.03	109.28
2	D	980	UDP	O3B-PB-O1B	-2.07	102.39	110.50
3	A	951[B]	UDC	O3-C3-C4	2.05	114.08	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	951[A]	UDC	O3-C3-C4	2.05	114.08	109.83
3	D	981[B]	UDC	O3-C3-C4	2.69	115.40	109.83
3	D	981[A]	UDC	O3-C3-C4	2.69	115.40	109.83
3	D	981[B]	UDC	C1-O5-C5	3.09	116.42	112.17
3	D	981[A]	UDC	C1-O5-C5	3.09	116.42	112.17
2	D	980	UDP	O3B-PB-O2B	3.21	120.58	107.61
2	B	960	UDP	O3B-PB-O2B	3.37	121.21	107.61
2	C	970	UDP	O3B-PB-O2B	3.45	121.54	107.61
2	A	950	UDP	O3B-PB-O2B	3.62	122.23	107.61
3	C	971[B]	UDC	C1-O5-C5	5.01	119.07	112.17
3	C	971[A]	UDC	C1-O5-C5	5.01	119.07	112.17
2	C	970	UDP	C4-N3-C2	5.48	118.84	114.13
2	B	960	UDP	C4-N3-C2	6.55	119.76	114.13
2	A	950	UDP	C4-N3-C2	6.97	120.12	114.13
2	D	980	UDP	C4-N3-C2	7.72	120.76	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	950	UDP	1	0
3	A	951[A]	UDC	4	0
3	B	961[A]	UDC	4	0
3	B	961[B]	UDC	1	0
3	C	971[A]	UDC	5	0
3	C	971[B]	UDC	4	0
3	D	981[A]	UDC	2	0
3	D	981[B]	UDC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2
1	D	2
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	67:IAS	CG	68:GLY	N	2.19
1	D	66:ARG	C	67:IAS	N	1.94
1	B	67:IAS	CG	68:GLY	N	1.82
1	A	66:ARG	C	67:IAS	N	1.76
1	C	66:ARG	C	67:IAS	N	1.74
1	C	67:IAS	CG	68:GLY	N	1.68
1	A	67:IAS	CG	68:GLY	N	1.65
1	B	66:ARG	C	67:IAS	N	1.61

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/423 (98%)	-0.09	4 (0%) 82 85	3, 9, 18, 29	0
1	B	417/423 (98%)	-0.22	2 (0%) 90 92	3, 10, 18, 32	0
1	C	417/423 (98%)	-0.26	4 (0%) 82 85	3, 10, 17, 28	0
1	D	417/423 (98%)	0.04	5 (1%) 79 81	2, 9, 17, 28	0
All	All	1668/1692 (98%)	-0.13	15 (0%) 84 86	2, 9, 18, 32	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.6
1	D	418	GLY	5.2
1	A	417	LYS	4.3
1	C	417	LYS	3.6
1	A	418	GLY	3.5
1	B	113	GLY	3.3
1	B	1	MET	3.2
1	D	68	GLY	2.9
1	C	322[A]	PHE	2.7
1	C	418	GLY	2.4
1	A	1	MET	2.3
1	D	86	LEU	2.2
1	D	148	ASP	2.2
1	C	252	ARG	2.2
1	A	246	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	IAS	B	67	8/9	0.87	0.15	-	14,14,15,16	0
1	IAS	D	67	8/9	0.84	0.14	-	14,15,16,18	0
1	IAS	A	67	8/9	0.98	0.06	-	8,8,9,9	0
1	IAS	C	67	8/9	0.84	0.11	-	4,6,7,8	0

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
3	UDC	D	981[A]	23/24	0.92	0.13	0.96	2,3,5,6	9
3	UDC	D	981[B]	23/24	0.92	0.13	0.81	2,2,5,6	9
3	UDC	A	951[B]	23/24	0.94	0.12	0.67	2,2,2,3	9
3	UDC	A	951[A]	23/24	0.94	0.12	0.40	2,2,2,3	9
3	UDC	C	971[A]	23/24	0.94	0.10	0.13	2,2,2,8	9
2	UDP	D	980	25/25	0.98	0.10	0.07	2,4,6,7	0
3	UDC	B	961[B]	23/24	0.95	0.11	0.02	2,2,2,2	9
2	UDP	C	970	25/25	0.97	0.10	0.02	2,2,7,10	0
3	UDC	B	961[A]	23/24	0.95	0.11	0.02	2,2,2,7	9
3	UDC	C	971[B]	23/24	0.94	0.10	-0.28	2,2,2,2	9
2	UDP	B	960	25/25	0.98	0.10	-0.29	2,2,4,5	0
2	UDP	A	950	25/25	0.98	0.08	-0.32	2,2,5,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.