Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 09:49 AM GMT

PDB ID	:	3JUK
Title	:	The Crystal Structure of UDP-glucose pyrophosphorylase complexed with UDP-glucose
Authors	:	Kim, H.; Kim, K.K.
Deposited on	:	2009-09-15
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

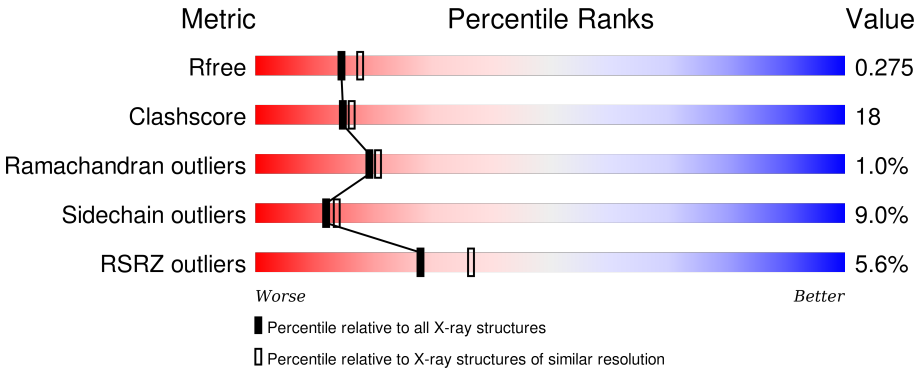
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	281	5% 66% 23% 5% 6%
1	B	281	4% 63% 25% 5% 6%
1	C	281	5% 63% 27% • 6%
1	D	281	6% 59% 30% 5% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9286 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-glucose pyrophosphorylase (GalU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2106	1343	352	397	14			
1	B	263	Total	C	N	O	S	0	0	0
			2091	1333	350	394	14			
1	C	264	Total	C	N	O	S	0	0	0
			2099	1339	351	395	14			
1	D	264	Total	C	N	O	S	0	0	0
			2098	1337	351	396	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	LEU	-	EXPRESSION TAG	UNP O25363
A	275	GLU	-	EXPRESSION TAG	UNP O25363
A	276	HIS	-	EXPRESSION TAG	UNP O25363
A	277	HIS	-	EXPRESSION TAG	UNP O25363
A	278	HIS	-	EXPRESSION TAG	UNP O25363
A	279	HIS	-	EXPRESSION TAG	UNP O25363
A	280	HIS	-	EXPRESSION TAG	UNP O25363
A	281	HIS	-	EXPRESSION TAG	UNP O25363
B	274	LEU	-	EXPRESSION TAG	UNP O25363
B	275	GLU	-	EXPRESSION TAG	UNP O25363
B	276	HIS	-	EXPRESSION TAG	UNP O25363
B	277	HIS	-	EXPRESSION TAG	UNP O25363
B	278	HIS	-	EXPRESSION TAG	UNP O25363
B	279	HIS	-	EXPRESSION TAG	UNP O25363
B	280	HIS	-	EXPRESSION TAG	UNP O25363
B	281	HIS	-	EXPRESSION TAG	UNP O25363
C	274	LEU	-	EXPRESSION TAG	UNP O25363
C	275	GLU	-	EXPRESSION TAG	UNP O25363
C	276	HIS	-	EXPRESSION TAG	UNP O25363
C	277	HIS	-	EXPRESSION TAG	UNP O25363
C	278	HIS	-	EXPRESSION TAG	UNP O25363

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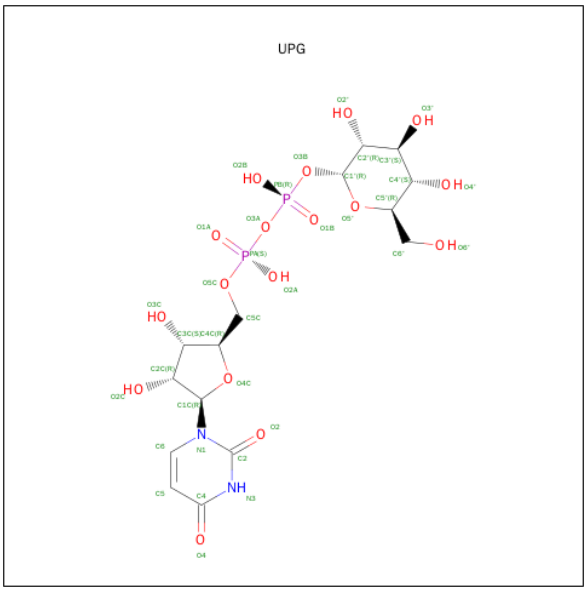
Chain	Residue	Modelled	Actual	Comment	Reference
C	279	HIS	-	EXPRESSION TAG	UNP O25363
C	280	HIS	-	EXPRESSION TAG	UNP O25363
C	281	HIS	-	EXPRESSION TAG	UNP O25363
D	274	LEU	-	EXPRESSION TAG	UNP O25363
D	275	GLU	-	EXPRESSION TAG	UNP O25363
D	276	HIS	-	EXPRESSION TAG	UNP O25363
D	277	HIS	-	EXPRESSION TAG	UNP O25363
D	278	HIS	-	EXPRESSION TAG	UNP O25363
D	279	HIS	-	EXPRESSION TAG	UNP O25363
D	280	HIS	-	EXPRESSION TAG	UNP O25363
D	281	HIS	-	EXPRESSION TAG	UNP O25363

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Mg 3 3	0	0
3	A	3	Total Mg 3 3	0	0
3	D	3	Total Mg 3 3	0	0
3	C	3	Total Mg 3 3	0	0

- Molecule 4 is water.

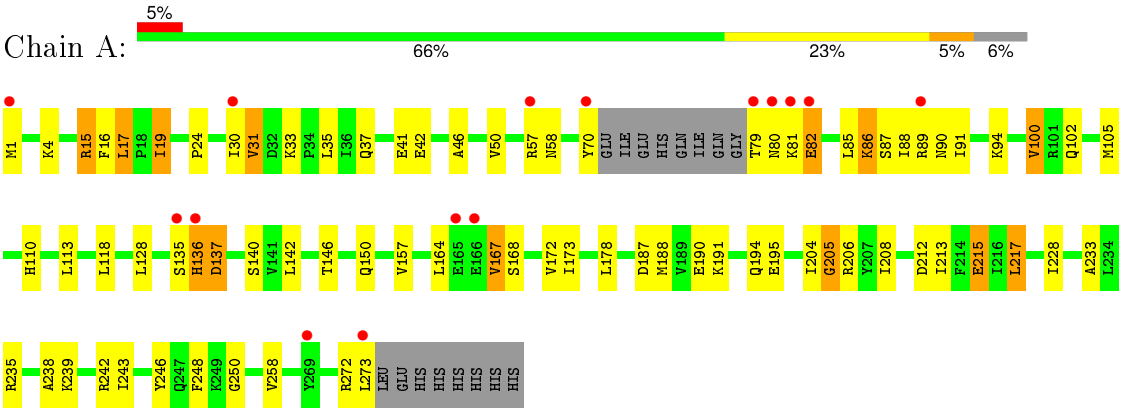
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	B	189	Total O 189 189	0	0
4	C	189	Total O 189 189	0	0
4	D	181	Total O 181 181	0	0

3 Residue-property plots (i)

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

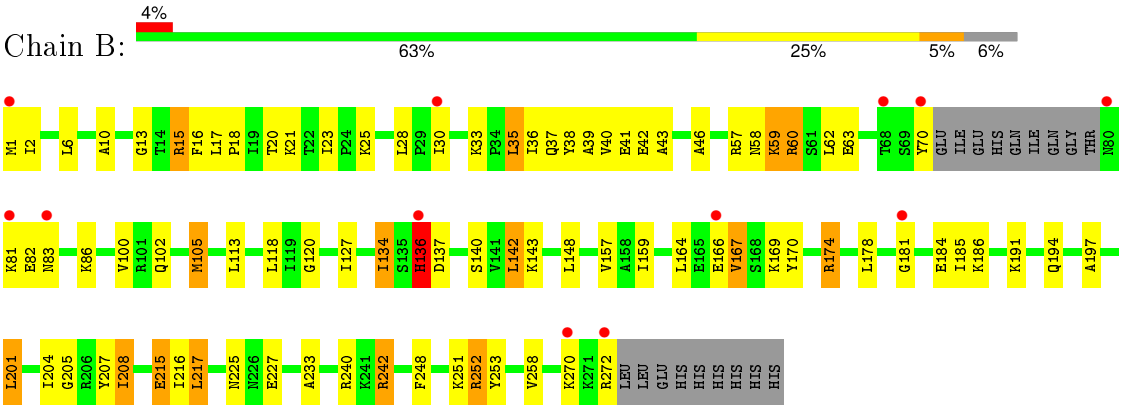
- Molecule 1: UDP-glucose pyrophosphorylase (GalU)

Chain A:



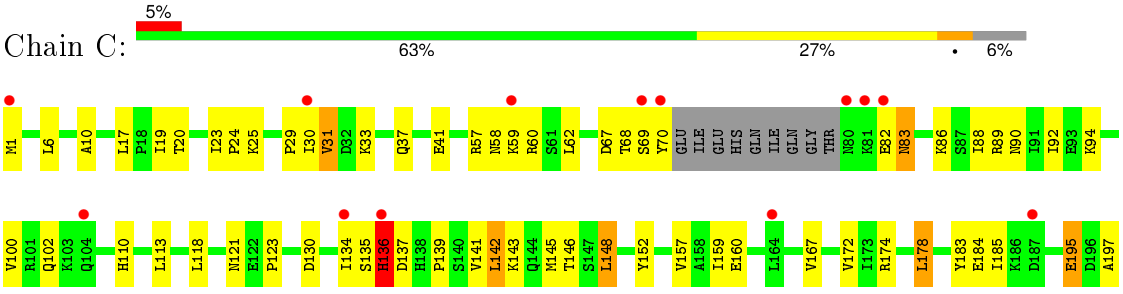
- Molecule 1: UDP-glucose pyrophosphorylase (GalU)

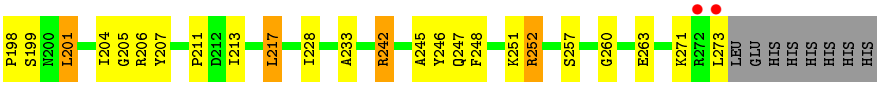
Chain B:



- Molecule 1: UDP-glucose pyrophosphorylase (GalU)

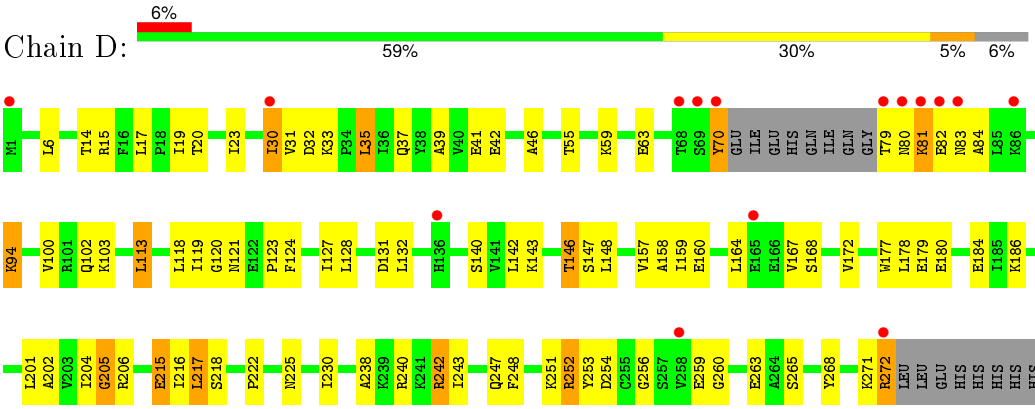
Chain C:





- Molecule 1: UDP-glucose pyrophosphorylase (GalU)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.44Å 74.39Å 167.12Å 90.00° 97.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 30.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	82.0 (50.00-2.30) 98.2 (30.02-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.276 0.258 , 0.275	Depositor DCC
R_{free} test set	2749 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	5 of 53953 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9286	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 84.93 % 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 1.4553e-07.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UPG, MG

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	0.41	0/2142	0.72	2/2885 (0.1%)
1	B	0.41	0/2127	0.70	2/2864 (0.1%)
1	C	0.41	0/2135	0.73	2/2875 (0.1%)
1	D	0.41	0/2134	0.72	2/2874 (0.1%)
All	All	0.41	0/8538	0.72	8/11498 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	174	ARG	N-CA-C	-5.76	95.44	111.00
1	A	137	ASP	N-CA-C	-5.64	95.76	111.00
1	B	208	ILE	N-CA-C	-5.55	96.02	111.00
1	A	208	ILE	N-CA-C	-5.38	96.49	111.00
1	D	81	LYS	N-CA-C	-5.18	97.00	111.00
1	D	30	ILE	N-CA-C	-5.05	97.35	111.00
1	C	6	LEU	CA-CB-CG	5.02	126.84	115.30
1	C	174	ARG	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2106	0	2145	69	0
1	B	2091	0	2127	75	1
1	C	2099	0	2138	81	0
1	D	2098	0	2134	89	0
2	A	36	0	21	2	0
2	B	36	0	21	2	0
2	C	36	0	21	2	0
2	D	36	0	21	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	177	0	0	3	0
4	B	189	0	0	9	0
4	C	189	0	0	8	1
4	D	181	0	0	13	0
All	All	9286	0	8628	304	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 18.

All (304) 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:102:GLN:HE22	2:C:283:UPG:HN3	1.02	1.01
1:C:70:TYR:HB2	1:C:89:ARG:HH22	1.25	1.00
1:D:79:THR:HG23	1:D:80:ASN:H	1.27	0.96
1:B:102:GLN:HE22	2:B:282:UPG:HN3	0.95	0.94
1:A:102:GLN:HE22	2:A:282:UPG:HN3	1.10	0.94
1:D:102:GLN:HE22	2:D:284:UPG:HN3	1.20	0.89
1:C:141:VAL:HG12	1:C:145:MET:HE1	1.57	0.87
1:A:164:LEU:HB3	1:A:194:GLN:NE2	1.90	0.86
1:D:242:ARG:HG3	1:D:242:ARG:HH11	1.40	0.85
1:A:90:ASN:HD21	1:A:94:LYS:HD3	1.41	0.84
1:C:70:TYR:HB2	1:C:89:ARG:NH2	1.92	0.84
1:C:139:PRO:HB3	1:C:143:LYS:HD3	1.57	0.84
1:D:242:ARG:NH1	1:D:242:ARG:HG3	1.94	0.83
1:A:42:GLU:HG3	1:A:140:SER:HB2	1.61	0.82
1:C:30:ILE:O	1:C:31:VAL:HG23	1.78	0.82
1:D:42:GLU:HG3	1:D:140:SER:HB2	1.62	0.81
1:B:136:HIS:CD2	1:B:136:HIS:H	1.97	0.80
1:D:272:ARG:HB3	1:D:272:ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ALA:HB2	1:A:243:ILE:HD11	1.64	0.80
1:D:242:ARG:CG	1:D:242:ARG:HH11	1.97	0.78
1:B:42:GLU:HG3	1:B:140:SER:HB2	1.65	0.78
1:A:90:ASN:ND2	1:A:94:LYS:HD3	1.98	0.78
1:A:136:HIS:CD2	1:A:136:HIS:H	2.02	0.76
1:D:238:ALA:HB2	1:D:243:ILE:HD11	1.68	0.76
1:C:167:VAL:HG13	1:C:172:VAL:HG21	1.67	0.76
1:A:15:ARG:HB3	1:A:15:ARG:NH2	2.01	0.76
1:A:15:ARG:HH21	1:A:15:ARG:HB3	1.51	0.75
1:A:30:ILE:O	1:A:31:VAL:HG23	1.85	0.75
1:B:37:GLN:O	1:B:41:GLU:HG3	1.87	0.75
1:B:60:ARG:HD2	1:B:60:ARG:H	1.52	0.74
1:A:136:HIS:HD2	1:A:136:HIS:H	1.36	0.74
1:C:195:GLU:HB2	4:C:286:HOH:O	1.88	0.73
1:A:164:LEU:HB3	1:A:194:GLN:HE21	1.51	0.73
1:B:59:LYS:HE2	1:B:63:GLU:OE2	1.89	0.72
1:C:141:VAL:HG12	1:C:145:MET:CE	2.19	0.72
1:C:19:ILE:HD11	1:C:23:ILE:HD12	1.70	0.72
1:D:89:ARG:O	1:D:93:GLU:HG2	1.90	0.70
1:D:79:THR:HG23	1:D:80:ASN:N	2.06	0.70
1:D:55:THR:HB	1:D:59:LYS:HB3	1.72	0.70
1:B:240:ARG:HD3	4:B:324:HOH:O	1.90	0.70
1:C:167:VAL:HG11	1:C:197:ALA:HB2	1.72	0.70
1:A:24:PRO:HD3	1:A:58:ASN:HB3	1.75	0.69
1:A:70:TYR:HE2	1:A:89:ARG:NH2	1.90	0.69
1:D:59:LYS:HD3	1:D:63:GLU:CD	2.14	0.69
1:C:90:ASN:HD21	1:C:94:LYS:NZ	1.92	0.68
1:B:136:HIS:HD2	1:B:136:HIS:H	1.41	0.68
1:B:1:MET:HA	4:B:633:HOH:O	1.94	0.68
1:A:235:ARG:NH2	1:A:239:LYS:HE3	2.09	0.68
1:D:55:THR:HG21	1:D:59:LYS:HE2	1.76	0.68
1:A:136:HIS:CD2	1:A:136:HIS:N	2.61	0.67
1:C:252:ARG:HD3	1:C:252:ARG:C	2.14	0.67
1:A:100:VAL:HG22	1:A:118:LEU:CD1	2.25	0.67
1:D:242:ARG:HA	4:D:318:HOH:O	1.95	0.66
1:C:90:ASN:HD21	1:C:94:LYS:HZ3	1.43	0.66
1:D:167:VAL:CG2	1:D:172:VAL:HG21	2.26	0.66
1:A:70:TYR:CE2	1:A:89:ARG:NH2	2.64	0.65
1:A:102:GLN:NE2	2:A:282:UPG:HN3	1.90	0.65
1:A:100:VAL:HG22	1:A:118:LEU:HD11	1.78	0.65
1:B:33:LYS:HE2	1:B:38:TYR:CE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:THR:HA	1:D:23:ILE:O	1.96	0.64
1:C:135:SER:O	1:C:137:ASP:N	2.31	0.64
1:A:167:VAL:HG12	4:A:541:HOH:O	1.96	0.64
1:A:167:VAL:HG22	1:A:172:VAL:HG21	1.79	0.64
1:A:15:ARG:HH21	1:A:15:ARG:CB	2.11	0.64
1:A:135:SER:HB3	1:A:250:GLY:HA3	1.78	0.64
1:C:29:PRO:HB3	1:D:19:ILE:HD13	1.79	0.64
1:A:16:PHE:O	1:A:19:ILE:HG22	1.98	0.63
1:D:14:THR:O	1:D:17:LEU:HB2	1.99	0.63
1:C:17:LEU:HD12	1:C:20:THR:OG1	1.99	0.63
1:B:134:ILE:HG23	1:B:251:LYS:HB3	1.81	0.62
1:B:20:THR:HA	1:B:23:ILE:O	1.99	0.62
1:B:100:VAL:HG13	1:B:118:LEU:HD21	1.81	0.62
1:A:33:LYS:HE3	1:A:37:GLN:HG2	1.80	0.62
1:D:102:GLN:NE2	2:D:284:UPG:HN3	1.95	0.62
1:B:217:LEU:HD13	1:B:233:ALA:HB2	1.83	0.61
1:C:167:VAL:HG11	1:C:197:ALA:CB	2.31	0.61
1:A:128:LEU:HB2	1:A:205:GLY:HA3	1.83	0.60
1:D:46:ALA:HA	1:D:143:LYS:HD3	1.83	0.59
1:B:217:LEU:HD13	1:B:233:ALA:CB	2.31	0.59
1:D:252:ARG:HD3	1:D:252:ARG:C	2.23	0.59
1:C:110:HIS:HB2	1:C:228:ILE:HD12	1.84	0.59
1:B:252:ARG:C	1:B:252:ARG:HD3	2.23	0.59
1:B:134:ILE:HD12	4:B:584:HOH:O	2.03	0.59
1:D:33:LYS:HD2	1:D:37:GLN:NE2	2.18	0.59
1:D:215:GLU:HG3	1:D:216:ILE:N	2.18	0.59
1:D:113:LEU:HG	1:D:217:LEU:HB3	1.85	0.59
1:C:113:LEU:HD11	4:C:551:HOH:O	2.01	0.58
1:C:102:GLN:NE2	2:C:283:UPG:HN3	1.87	0.58
1:C:142:LEU:HA	1:C:145:MET:HE2	1.86	0.58
1:B:10:ALA:HB3	1:B:102:GLN:NE2	2.18	0.58
1:A:128:LEU:HD22	1:A:205:GLY:HA2	1.85	0.58
1:D:184:GLU:OE1	1:D:242:ARG:NH1	2.37	0.58
1:B:136:HIS:CD2	1:B:136:HIS:N	2.71	0.58
1:D:167:VAL:HG22	1:D:172:VAL:HG21	1.85	0.58
1:D:131:ASP:O	1:D:206:ARG:NH1	2.36	0.58
1:B:57:ARG:NH1	1:C:68:THR:OG1	2.37	0.57
1:D:128:LEU:HD22	1:D:205:GLY:HA2	1.86	0.57
1:B:10:ALA:HB3	1:B:102:GLN:HE21	1.69	0.57
1:D:247:GLN:NE2	4:D:360:HOH:O	2.37	0.57
1:A:70:TYR:HD2	1:A:89:ARG:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:HD21	1:A:94:LYS:CD	2.15	0.57
1:D:80:ASN:O	1:D:84:ALA:HB2	2.04	0.56
1:A:100:VAL:HG22	1:A:118:LEU:HG	1.87	0.56
1:D:128:LEU:HG	2:D:284:UPG:H4C	1.88	0.56
1:D:70:TYR:CD2	1:D:70:TYR:C	2.78	0.56
1:B:169:LYS:HE3	1:B:170:TYR:CZ	2.41	0.56
1:B:174:ARG:NH1	1:B:186:LYS:HB3	2.20	0.56
1:C:29:PRO:HB3	1:D:19:ILE:CD1	2.37	0.55
1:A:100:VAL:HG22	1:A:118:LEU:CG	2.37	0.55
1:B:60:ARG:N	1:B:60:ARG:HD2	2.20	0.55
1:C:157:VAL:HG22	1:C:185:ILE:HD11	1.89	0.55
1:C:242:ARG:HG3	1:C:242:ARG:HH21	1.70	0.55
1:C:17:LEU:CD2	1:D:81:LYS:HG3	2.37	0.54
1:A:81:LYS:HB3	1:A:85:LEU:HD12	1.89	0.54
1:D:120:GLY:HA3	4:D:568:HOH:O	2.05	0.54
1:B:167:VAL:HG11	1:B:197:ALA:HB2	1.89	0.54
1:B:105:MET:O	1:B:105:MET:HG3	2.07	0.54
1:D:238:ALA:HB2	1:D:243:ILE:CD1	2.37	0.54
1:A:212:ASP:O	1:A:215:GLU:HG3	2.07	0.54
1:A:94:LYS:NZ	4:A:717:HOH:O	2.41	0.54
1:B:36:ILE:O	1:B:40:VAL:HG23	2.08	0.54
1:A:81:LYS:HA	1:B:17:LEU:HD23	1.90	0.54
1:B:215:GLU:HG3	1:B:216:ILE:N	2.23	0.54
1:C:217:LEU:HD13	1:C:233:ALA:HB2	1.88	0.54
1:B:252:ARG:HD3	1:B:253:TYR:N	2.23	0.53
1:A:87:SER:O	1:A:91:ILE:HG13	2.08	0.53
1:B:33:LYS:HE2	1:B:38:TYR:CZ	2.44	0.53
1:C:184:GLU:OE1	1:C:242:ARG:NH2	2.42	0.53
1:C:20:THR:HA	1:C:23:ILE:O	2.09	0.53
1:C:184:GLU:OE1	1:C:242:ARG:HG3	2.08	0.53
1:B:82:GLU:O	1:B:86:LYS:HG3	2.09	0.53
1:D:225:ASN:HB3	4:D:664:HOH:O	2.09	0.53
1:B:25:LYS:HA	1:B:28:LEU:HG	1.90	0.53
1:A:235:ARG:CZ	1:A:239:LYS:HE3	2.39	0.52
1:C:183:TYR:HE1	1:C:247:GLN:HE21	1.57	0.52
1:B:252:ARG:C	1:B:252:ARG:CD	2.78	0.52
1:A:46:ALA:CB	1:A:142:LEU:HD12	2.38	0.52
1:B:13:GLY:O	1:B:20:THR:HG21	2.09	0.52
1:A:57:ARG:HH22	1:B:70:TYR:C	2.13	0.52
1:D:31:VAL:HG23	1:D:32:ASP:N	2.24	0.52
1:B:136:HIS:CG	1:B:137:ASP:H	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:CG2	1:C:251:LYS:HB3	2.40	0.52
1:C:100:VAL:HG13	1:C:118:LEU:HD21	1.91	0.52
1:B:43:ALA:HA	1:B:142:LEU:HD12	1.90	0.52
1:B:143:LYS:HE2	4:B:349:HOH:O	2.10	0.52
1:D:100:VAL:HG13	1:D:118:LEU:HD21	1.90	0.52
1:A:37:GLN:O	1:A:41:GLU:HG3	2.10	0.52
1:C:178:LEU:HD21	1:C:184:GLU:HB2	1.92	0.52
1:A:213:ILE:O	1:A:217:LEU:HD22	2.09	0.52
1:D:251:LYS:HD2	4:D:356:HOH:O	2.09	0.52
1:B:2:ILE:CD1	1:B:208:ILE:HD12	2.40	0.52
1:C:69:SER:OG	1:C:70:TYR:N	2.41	0.51
1:D:79:THR:CG2	1:D:80:ASN:H	2.12	0.51
1:B:184:GLU:OE1	1:B:242:ARG:HD3	2.10	0.51
1:C:83:ASN:HA	1:C:86:LYS:HE2	1.90	0.51
1:B:60:ARG:H	1:B:60:ARG:CD	2.14	0.51
1:B:166:GLU:OE1	1:B:169:LYS:HE2	2.10	0.51
1:A:238:ALA:HB2	1:A:243:ILE:CD1	2.37	0.51
1:B:17:LEU:CD1	1:B:20:THR:HG23	2.40	0.51
1:A:33:LYS:HE3	1:A:37:GLN:CG	2.41	0.51
1:D:31:VAL:HG22	1:D:268:TYR:CE2	2.45	0.51
1:C:260:GLY:HA2	1:C:263:GLU:HG2	1.93	0.51
1:C:142:LEU:HA	1:C:145:MET:CE	2.40	0.51
1:B:10:ALA:CB	1:B:102:GLN:HE21	2.24	0.51
1:A:238:ALA:HA	1:A:243:ILE:HG12	1.93	0.51
1:B:63:GLU:OE1	1:C:59:LYS:HD3	2.10	0.51
1:B:240:ARG:HD2	4:B:300:HOH:O	2.11	0.50
1:C:242:ARG:HG3	1:C:242:ARG:NH2	2.24	0.50
1:C:33:LYS:HE3	1:C:37:GLN:NE2	2.28	0.49
1:C:145:MET:CE	1:C:206:ARG:HB3	2.42	0.49
4:C:570:HOH:O	1:D:259:GLU:HB2	2.11	0.49
1:A:42:GLU:HG3	1:A:140:SER:CB	2.35	0.49
1:B:83:ASN:HA	1:B:86:LYS:HD3	1.95	0.49
1:C:100:VAL:HG22	1:C:118:LEU:HD11	1.95	0.49
1:C:136:HIS:HE1	1:C:271:LYS:NZ	2.11	0.48
1:C:204:ILE:HG22	1:C:252:ARG:NH1	2.29	0.48
1:D:39:ALA:HB1	1:D:127:ILE:HG21	1.96	0.48
1:D:15:ARG:HD2	1:D:256:GLY:O	2.13	0.48
1:D:100:VAL:HG22	1:D:118:LEU:HD11	1.96	0.48
1:A:205:GLY:O	1:A:206:ARG:HD3	2.14	0.48
1:D:37:GLN:O	1:D:41:GLU:HG3	2.14	0.48
1:A:4:LYS:HG2	1:A:50:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:LYS:HG3	4:D:338:HOH:O	2.14	0.47
1:D:230:ILE:HG22	4:D:316:HOH:O	2.14	0.47
1:D:30:ILE:HD11	1:D:35:LEU:CD1	2.44	0.47
1:B:157:VAL:O	1:B:157:VAL:HG23	2.15	0.47
1:B:204:ILE:HD13	1:B:248:PHE:CE2	2.49	0.47
1:B:18:PRO:O	1:B:21:LYS:HB3	2.14	0.47
1:D:31:VAL:CG2	1:D:32:ASP:N	2.77	0.47
1:D:194:GLN:HG3	4:D:687:HOH:O	2.14	0.47
1:B:17:LEU:HD13	1:B:20:THR:HG23	1.96	0.46
1:B:159:ILE:HD12	1:B:201:LEU:HG	1.97	0.46
1:D:164:LEU:O	1:D:167:VAL:HG12	2.15	0.46
1:D:80:ASN:O	1:D:84:ALA:CB	2.64	0.46
1:D:31:VAL:CG2	1:D:268:TYR:CE2	2.98	0.46
1:D:240:ARG:NH2	4:D:628:HOH:O	2.49	0.46
1:D:42:GLU:HG3	1:D:140:SER:CB	2.41	0.46
1:C:242:ARG:CG	1:C:242:ARG:HH21	2.29	0.46
1:B:105:MET:O	1:B:105:MET:CG	2.63	0.46
1:B:30:ILE:HD11	1:B:35:LEU:CD1	2.46	0.45
1:C:25:LYS:HE3	1:C:130:ASP:HB3	1.99	0.45
1:C:88:ILE:O	1:C:92:ILE:HG13	2.15	0.45
1:D:177:TRP:CH2	1:D:179:GLU:HA	2.50	0.45
1:B:240:ARG:CD	4:B:300:HOH:O	2.63	0.45
1:C:10:ALA:HB3	1:C:102:GLN:HE21	1.82	0.45
1:C:157:VAL:CG2	1:C:185:ILE:HD11	2.46	0.45
1:C:83:ASN:HD22	1:C:83:ASN:HA	1.59	0.45
1:B:58:ASN:ND2	4:B:357:HOH:O	2.49	0.45
1:C:24:PRO:HG3	1:C:58:ASN:HB2	1.98	0.45
1:D:252:ARG:CD	1:D:252:ARG:C	2.84	0.45
1:B:184:GLU:OE1	1:B:242:ARG:CD	2.65	0.45
1:C:204:ILE:HD13	1:C:248:PHE:CE2	2.51	0.45
1:B:270:LYS:HA	1:B:272:ARG:NH2	2.32	0.44
1:C:134:ILE:HG23	1:C:251:LYS:HB3	1.98	0.44
1:D:254:ASP:O	1:D:260:GLY:HA3	2.18	0.44
1:C:59:LYS:HE3	4:C:511:HOH:O	2.17	0.44
1:A:88:ILE:HA	1:A:91:ILE:HD12	1.98	0.44
1:D:31:VAL:CG2	1:D:268:TYR:HE2	2.30	0.44
1:C:141:VAL:O	1:C:145:MET:HE2	2.18	0.44
1:D:272:ARG:CB	1:D:272:ARG:HH11	2.23	0.44
1:B:1:MET:HA	4:B:587:HOH:O	2.18	0.44
1:A:33:LYS:CE	1:A:37:GLN:HG2	2.46	0.44
1:D:148:LEU:HA	1:D:148:LEU:HD23	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:CD2	1:B:81:LYS:HG3	2.48	0.44
1:C:159:ILE:O	1:C:247:GLN:HA	2.18	0.44
1:C:82:GLU:HB2	4:C:302:HOH:O	2.17	0.44
1:D:30:ILE:HG22	1:D:265:SER:HA	2.00	0.43
1:D:159:ILE:HA	1:D:202:ALA:O	2.18	0.43
1:C:157:VAL:O	1:C:245:ALA:HA	2.19	0.43
1:C:57:ARG:NH2	4:C:380:HOH:O	2.51	0.43
1:A:204:ILE:HD13	1:A:248:PHE:CE2	2.54	0.43
1:B:102:GLN:NE2	2:B:282:UPG:HN3	1.81	0.43
1:A:100:VAL:CG2	1:A:118:LEU:CD1	2.96	0.43
1:A:135:SER:HB3	1:A:250:GLY:CA	2.46	0.43
1:D:123:PRO:HD2	4:D:599:HOH:O	2.18	0.43
1:A:33:LYS:HE3	1:A:37:GLN:CD	2.39	0.43
1:C:37:GLN:O	1:C:41:GLU:HG3	2.18	0.43
1:B:186:LYS:HE2	1:B:186:LYS:HA	2.01	0.43
1:A:272:ARG:CZ	1:B:258:VAL:HG21	2.49	0.43
1:D:178:LEU:HD21	1:D:242:ARG:NH2	2.34	0.42
1:A:86:LYS:NZ	4:A:716:HOH:O	2.52	0.42
1:C:148:LEU:HD22	1:C:152:TYR:CD2	2.54	0.42
1:D:80:ASN:HA	1:D:83:ASN:HB2	2.01	0.42
1:D:80:ASN:CG	1:D:80:ASN:O	2.57	0.42
1:D:184:GLU:HG3	1:D:242:ARG:HG3	2.01	0.42
1:C:246:TYR:CE2	1:C:248:PHE:HA	2.55	0.42
1:B:225:ASN:O	1:B:227:GLU:HG3	2.19	0.42
1:C:204:ILE:HG22	1:C:252:ARG:HH12	1.83	0.42
1:C:136:HIS:HE1	1:C:271:LYS:HZ3	1.67	0.42
1:B:39:ALA:HB1	1:B:127:ILE:HG21	2.00	0.42
1:B:120:GLY:HA3	4:B:365:HOH:O	2.20	0.42
1:A:70:TYR:HE2	1:A:89:ARG:HH21	1.59	0.42
1:C:213:ILE:O	1:C:217:LEU:HD22	2.19	0.42
1:D:146:THR:HG22	1:D:147:SER:N	2.34	0.42
1:D:158:ALA:CB	1:D:206:ARG:HB2	2.50	0.42
1:C:159:ILE:HD12	1:C:201:LEU:HG	2.02	0.42
1:D:222:PRO:HB2	4:D:634:HOH:O	2.18	0.42
1:C:70:TYR:HD2	1:C:89:ARG:HH21	1.66	0.42
1:C:198:PRO:O	1:C:199:SER:HB3	2.17	0.42
1:B:17:LEU:HD13	1:B:20:THR:CG2	2.50	0.42
1:C:252:ARG:O	1:C:252:ARG:HD3	2.20	0.42
1:D:252:ARG:HD3	1:D:253:TYR:N	2.35	0.42
1:C:271:LYS:C	1:C:273:LEU:N	2.72	0.41
1:C:160:GLU:HG3	4:C:383:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ILE:HD13	1:D:248:PHE:CZ	2.55	0.41
1:D:132:LEU:HA	4:D:292:HOH:O	2.19	0.41
1:D:215:GLU:O	1:D:218:SER:HB2	2.21	0.41
1:A:272:ARG:NH2	1:B:258:VAL:HG21	2.35	0.41
1:A:79:THR:N	1:A:82:GLU:HB3	2.36	0.41
1:D:90:ASN:O	1:D:94:LYS:HB2	2.21	0.41
1:D:100:VAL:HG22	1:D:118:LEU:CD1	2.49	0.41
1:B:46:ALA:HB2	1:B:142:LEU:HB3	2.03	0.41
1:D:204:ILE:HD13	1:D:248:PHE:CE2	2.56	0.41
1:C:271:LYS:C	1:C:273:LEU:H	2.23	0.41
1:C:60:ARG:HA	1:C:60:ARG:HE	1.85	0.41
1:C:1:MET:HG2	4:C:574:HOH:O	2.20	0.41
1:B:169:LYS:HE3	1:B:170:TYR:OH	2.21	0.41
1:A:217:LEU:HD13	1:A:233:ALA:CB	2.50	0.41
1:D:242:ARG:CB	1:D:242:ARG:HH11	2.33	0.41
1:D:242:ARG:HG2	1:D:243:ILE:N	2.36	0.41
1:A:70:TYR:CD2	1:A:85:LEU:HD13	2.56	0.41
1:D:253:TYR:CE2	1:D:263:GLU:HG2	2.56	0.41
1:B:169:LYS:HE3	1:B:170:TYR:CE1	2.55	0.41
1:C:100:VAL:HG13	1:C:118:LEU:CD2	2.51	0.41
1:D:177:TRP:CZ2	1:D:179:GLU:C	2.94	0.41
1:A:246:TYR:CE2	1:A:248:PHE:HA	2.56	0.41
1:A:190:GLU:HG3	1:A:191:LYS:HG3	2.01	0.41
1:B:15:ARG:HB3	1:B:16:PHE:CD1	2.56	0.41
1:A:187:ASP:OD2	1:A:188:MET:N	2.51	0.41
1:D:164:LEU:HA	1:D:164:LEU:HD23	1.95	0.41
1:B:157:VAL:HG22	1:B:185:ILE:HD11	2.03	0.41
1:D:186:LYS:HE2	4:D:434:HOH:O	2.21	0.41
1:C:145:MET:HE1	1:C:206:ARG:HB3	2.03	0.40
1:C:167:VAL:HG13	1:C:172:VAL:CG2	2.43	0.40
1:A:217:LEU:HD13	1:A:233:ALA:HB2	2.02	0.40
1:B:157:VAL:O	1:B:157:VAL:CG2	2.69	0.40
1:A:110:HIS:HB2	1:A:228:ILE:HD12	2.03	0.40
1:C:123:PRO:CA	1:C:211:PRO:HD3	2.51	0.40
1:D:119:ILE:HG21	1:D:124:PHE:CD2	2.56	0.40
1:C:123:PRO:HA	1:C:211:PRO:HD3	2.03	0.40
1:D:93:GLU:HG2	1:D:93:GLU:H	1.77	0.40
1:D:168:SER:HA	1:D:192:PRO:O	2.22	0.40
1:A:30:ILE:HA	1:A:30:ILE:HD13	1.82	0.40
1:A:173:ILE:HG13	1:A:173:ILE:O	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLY:N	4:C:454:HOH:O[1_565]	2.14	0.06

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	261/281 (93%)	245 (94%)	13 (5%)	3 (1%)	17	18
1	B	259/281 (92%)	244 (94%)	13 (5%)	2 (1%)	24	27
1	C	260/281 (92%)	245 (94%)	12 (5%)	3 (1%)	16	16
1	D	260/281 (92%)	249 (96%)	9 (4%)	2 (1%)	24	27
All	All	1040/1124 (92%)	983 (94%)	47 (4%)	10 (1%)	19	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	82	GLU
1	B	136	HIS
1	C	31	VAL
1	C	136	HIS
1	A	205	GLY
1	C	205	GLY
1	D	180	GLU
1	B	205	GLY
1	D	205	GLY

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	229/244 (94%)	205 (90%)	24 (10%)	8 9
1	B	227/244 (93%)	204 (90%)	23 (10%)	9 11
1	C	228/244 (93%)	212 (93%)	16 (7%)	19 23
1	D	228/244 (93%)	209 (92%)	19 (8%)	14 17
All	All	912/976 (93%)	830 (91%)	82 (9%)	12 14

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	ARG
1	A	17	LEU
1	A	19	ILE
1	A	35	LEU
1	A	80	ASN
1	A	86	LYS
1	A	100	VAL
1	A	105	MET
1	A	113	LEU
1	A	136	HIS
1	A	137	ASP
1	A	146	THR
1	A	150	GLN
1	A	157	VAL
1	A	167	VAL
1	A	168	SER
1	A	178	LEU
1	A	195	GLU
1	A	215	GLU
1	A	217	LEU
1	A	242	ARG
1	A	258	VAL
1	A	273	LEU
1	B	6	LEU
1	B	15	ARG
1	B	35	LEU
1	B	59	LYS

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Mol	Chain	Res	Type
1	B	60	ARG
1	B	62	LEU
1	B	105	MET
1	B	113	LEU
1	B	134	ILE
1	B	136	HIS
1	B	142	LEU
1	B	148	LEU
1	B	164	LEU
1	B	167	VAL
1	B	178	LEU
1	B	191	LYS
1	B	194	GLN
1	B	201	LEU
1	B	207	TYR
1	B	215	GLU
1	B	217	LEU
1	B	242	ARG
1	B	252	ARG
1	C	62	LEU
1	C	67	ASP
1	C	83	ASN
1	C	121	ASN
1	C	136	HIS
1	C	142	LEU
1	C	146	THR
1	C	148	LEU
1	C	178	LEU
1	C	195	GLU
1	C	201	LEU
1	C	207	TYR
1	C	217	LEU
1	C	242	ARG
1	C	252	ARG
1	C	257	SER
1	D	6	LEU
1	D	35	LEU
1	D	70	TYR
1	D	82	GLU
1	D	94	LYS
1	D	113	LEU
1	D	121	ASN

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Mol	Chain	Res	Type
1	D	142	LEU
1	D	146	THR
1	D	157	VAL
1	D	160	GLU
1	D	195	GLU
1	D	201	LEU
1	D	215	GLU
1	D	217	LEU
1	D	242	ARG
1	D	252	ARG
1	D	271	LYS
1	D	272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	58	ASN
1	A	83	ASN
1	A	90	ASN
1	A	102	GLN
1	A	136	HIS
1	A	193	ASN
1	A	194	GLN
1	A	226	ASN
1	A	247	GLN
1	A	266	ASN
1	B	80	ASN
1	B	83	ASN
1	B	90	ASN
1	B	102	GLN
1	B	136	HIS
1	B	266	ASN
1	C	58	ASN
1	C	83	ASN
1	C	90	ASN
1	C	102	GLN
1	C	121	ASN
1	C	136	HIS
1	C	150	GLN
1	C	193	ASN
1	C	247	GLN

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Mol	Chain	Res	Type
1	D	102	GLN
1	D	121	ASN
1	D	150	GLN
1	D	153	GLN
1	D	194	GLN
1	D	229	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UPG	A	282	3	29,38,38	1.78	7 (24%)	43,58,58	1.45	3 (6%)
2	UPG	B	282	3	29,38,38	1.78	7 (24%)	43,58,58	1.48	3 (6%)
2	UPG	C	283	3	29,38,38	1.71	7 (24%)	43,58,58	1.42	3 (6%)
2	UPG	D	284	3	29,38,38	1.76	8 (27%)	43,58,58	1.42	3 (6%)

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	UPG	A	282	3	-	0/19/59/59	0/3/3/3
2	UPG	B	282	3	-	0/19/59/59	0/3/3/3
2	UPG	C	283	3	-	0/19/59/59	0/3/3/3
2	UPG	D	284	3	-	0/19/59/59	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	282	UPG	PA-O1A	-4.44	1.35	1.51
2	D	284	UPG	PA-O1A	-4.31	1.35	1.51
2	A	282	UPG	PA-O1A	-4.24	1.35	1.51
2	C	283	UPG	PA-O1A	-4.15	1.36	1.51
2	C	283	UPG	PA-O2A	-3.68	1.39	1.54
2	B	282	UPG	PB-O2B	-3.62	1.39	1.54
2	A	282	UPG	PA-O2A	-3.56	1.39	1.54
2	C	283	UPG	PB-O2B	-3.47	1.40	1.54
2	B	282	UPG	PA-O2A	-3.37	1.40	1.54
2	D	284	UPG	PB-O2B	-3.33	1.40	1.54
2	A	282	UPG	PB-O2B	-3.27	1.41	1.54
2	D	284	UPG	PA-O2A	-3.20	1.41	1.54
2	D	284	UPG	PB-O1B	-3.01	1.40	1.51
2	B	282	UPG	PB-O1B	-2.99	1.40	1.51
2	B	282	UPG	O4-C4	-2.88	1.17	1.24
2	A	282	UPG	O4C-C4C	-2.87	1.38	1.45
2	D	284	UPG	O4C-C4C	-2.80	1.38	1.45
2	A	282	UPG	PB-O1B	-2.77	1.41	1.51
2	C	283	UPG	PB-O1B	-2.61	1.41	1.51
2	D	284	UPG	O4-C4	-2.51	1.18	1.24
2	C	283	UPG	O4C-C4C	-2.50	1.39	1.45
2	A	282	UPG	O4-C4	-2.45	1.18	1.24
2	C	283	UPG	O4-C4	-2.43	1.18	1.24
2	B	282	UPG	O4C-C4C	-2.34	1.39	1.45
2	D	284	UPG	PB-O3B	-2.10	1.54	1.60
2	A	282	UPG	PA-O5C	-2.10	1.49	1.59
2	D	284	UPG	O3'-C3'	-2.07	1.38	1.43
2	C	283	UPG	O3'-C3'	-2.04	1.38	1.43
2	B	282	UPG	O3'-C3'	-2.04	1.38	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	283	UPG	O3C-C3C-C4C	-2.54	103.43	111.05
2	A	282	UPG	O3C-C3C-C4C	-2.54	103.45	111.05
2	B	282	UPG	O3C-C3C-C4C	-2.52	103.49	111.05
2	D	284	UPG	O3C-C3C-C4C	-2.24	104.33	111.05
2	D	284	UPG	O4'-C4'-C3'	2.26	115.41	110.34
2	C	283	UPG	O4'-C4'-C3'	2.51	116.00	110.34
2	B	282	UPG	O4'-C4'-C3'	2.70	116.41	110.34
2	A	282	UPG	O4'-C4'-C3'	2.70	116.43	110.34
2	C	283	UPG	C4-N3-C2	6.26	120.34	114.14
2	A	282	UPG	C4-N3-C2	6.33	120.42	114.14
2	D	284	UPG	C4-N3-C2	6.67	120.75	114.14
2	B	282	UPG	C4-N3-C2	6.69	120.77	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	282	UPG	2	0
2	B	282	UPG	2	0
2	C	283	UPG	2	0
2	D	284	UPG	3	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^{th} 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	265/281 (94%)	0.49	15 (5%)	27	36	10, 23, 42, 60	0
1	B	263/281 (93%)	0.45	12 (4%)	36	45	8, 22, 40, 58	0
1	C	264/281 (93%)	0.45	15 (5%)	27	36	12, 22, 41, 65	0
1	D	264/281 (93%)	0.49	17 (6%)	23	31	11, 24, 41, 67	0
All	All	1056/1124 (93%)	0.47	59 (5%)	28	36	8, 23, 41, 67	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	80	ASN	8.2
1	A	79	THR	7.3
1	A	70	TYR	6.4
1	D	70	TYR	5.7
1	D	79	THR	5.7
1	C	69	SER	5.4
1	A	80	ASN	5.4
1	B	80	ASN	5.0
1	B	70	TYR	4.8
1	C	136	HIS	4.5
1	C	80	ASN	4.5
1	D	136	HIS	4.4
1	D	69	SER	3.9
1	C	70	TYR	3.9
1	B	1	MET	3.8
1	D	30	ILE	3.7
1	A	136	HIS	3.7
1	A	135	SER	3.6
1	A	30	ILE	3.5
1	C	81	LYS	3.4
1	D	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	81	LYS	3.4
1	A	1	MET	3.4
1	D	82	GLU	3.1
1	D	68	THR	3.1
1	C	30	ILE	3.1
1	B	30	ILE	3.0
1	C	134	ILE	2.8
1	B	136	HIS	2.8
1	B	68	THR	2.8
1	A	57	ARG	2.7
1	C	1	MET	2.7
1	A	89	ARG	2.6
1	B	166	GLU	2.6
1	D	83	ASN	2.6
1	A	81	LYS	2.6
1	D	165	GLU	2.5
1	C	272	ARG	2.5
1	A	82	GLU	2.4
1	A	165	GLU	2.4
1	B	83	ASN	2.4
1	C	82	GLU	2.4
1	C	59	LYS	2.3
1	C	273	LEU	2.3
1	D	193	ASN	2.3
1	B	81	LYS	2.2
1	A	166	GLU	2.2
1	D	93	GLU	2.2
1	B	181	GLY	2.2
1	B	270	LYS	2.1
1	D	258	VAL	2.1
1	D	86	LYS	2.1
1	A	273	LEU	2.1
1	B	272	ARG	2.1
1	C	187	ASP	2.0
1	D	272	ARG	2.0
1	C	164	LEU	2.0
1	C	104	GLN	2.0
1	A	269	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	UPG	C	283	36/36	0.95	0.13	-0.75	13,17,20,21	0
2	UPG	D	284	36/36	0.95	0.13	-1.02	15,19,22,24	0
2	UPG	A	282	36/36	0.95	0.12	-1.06	12,17,21,22	0
2	UPG	B	282	36/36	0.96	0.12	-1.29	13,16,20,22	0
3	MG	D	312	1/1	0.79	0.36	-	28,28,28,28	0
3	MG	C	309	1/1	0.79	0.30	-	25,25,25,25	0
3	MG	C	308	1/1	0.97	0.30	-	26,26,26,26	0
3	MG	B	304	1/1	0.96	0.20	-	36,36,36,36	0
3	MG	A	301	1/1	0.88	0.18	-	28,28,28,28	0
3	MG	B	306	1/1	0.98	0.33	-	31,31,31,31	0
3	MG	D	310	1/1	0.69	0.20	-	35,35,35,35	0
3	MG	B	305	1/1	0.88	0.32	-	33,33,33,33	0
3	MG	A	303	1/1	0.91	0.27	-	31,31,31,31	0
3	MG	A	302	1/1	0.90	0.26	-	20,20,20,20	0
3	MG	C	307	1/1	0.92	0.14	-	19,19,19,19	0
3	MG	D	311	1/1	0.87	0.38	-	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.