Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 11:25 PM EST

PDB ID	:	3JUJ
Title	:	The crystal structure of apo- UDP-glucose pyrophosphorylase
Authors	:	Kim, H.; Kim, K.K.
Deposited on	:	2009-09-15
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

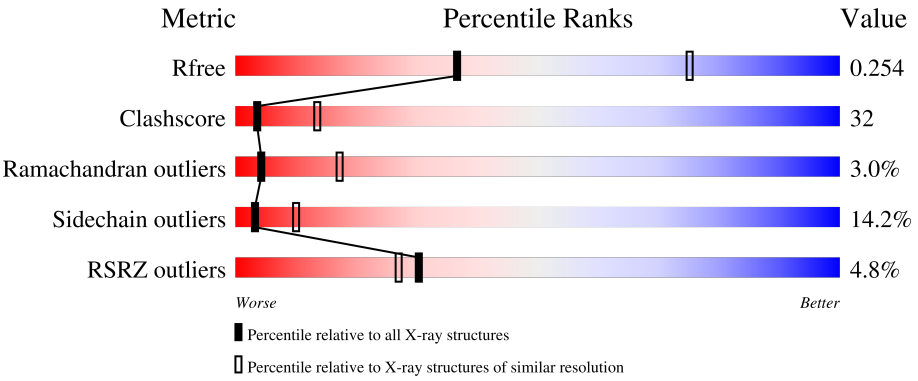
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 49% 37% 10%
1	B	281	5% 46% 39% 11%
1	C	281	6% 48% 39% 10%
1	D	281	5% 48% 40% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8783 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	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	14			
1	B	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	14			
1	C	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	14			
1	D	273	Total	C	N	O	S	0	0	0
			2172	1383	364	411	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

Continued on next page...

Continued from previous page...

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 water.

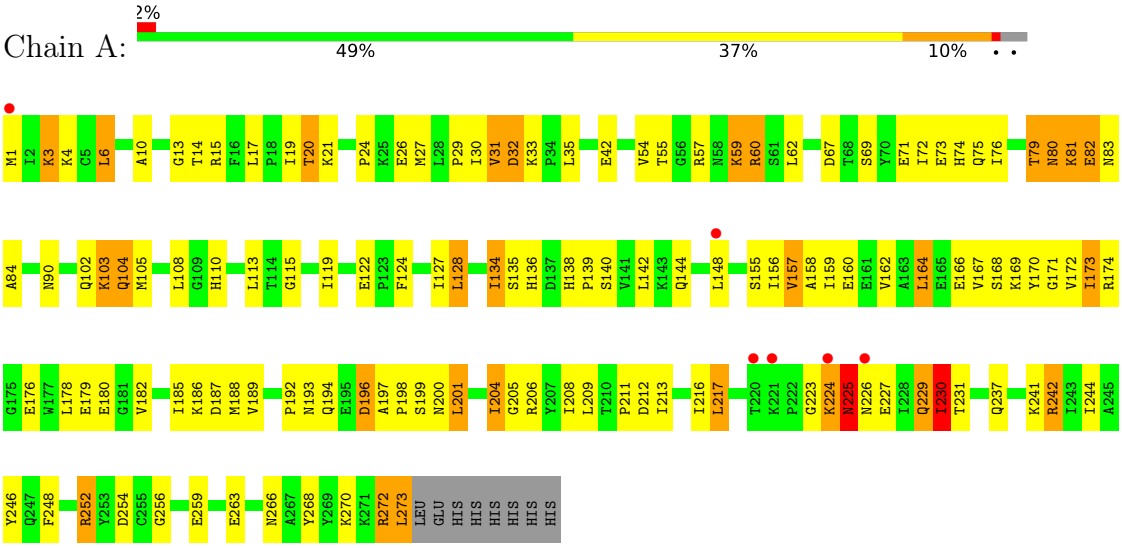
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	24	Total O 24 24	0	0
2	C	30	Total O 30 30	0	0
2	D	21	Total O 21 21	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

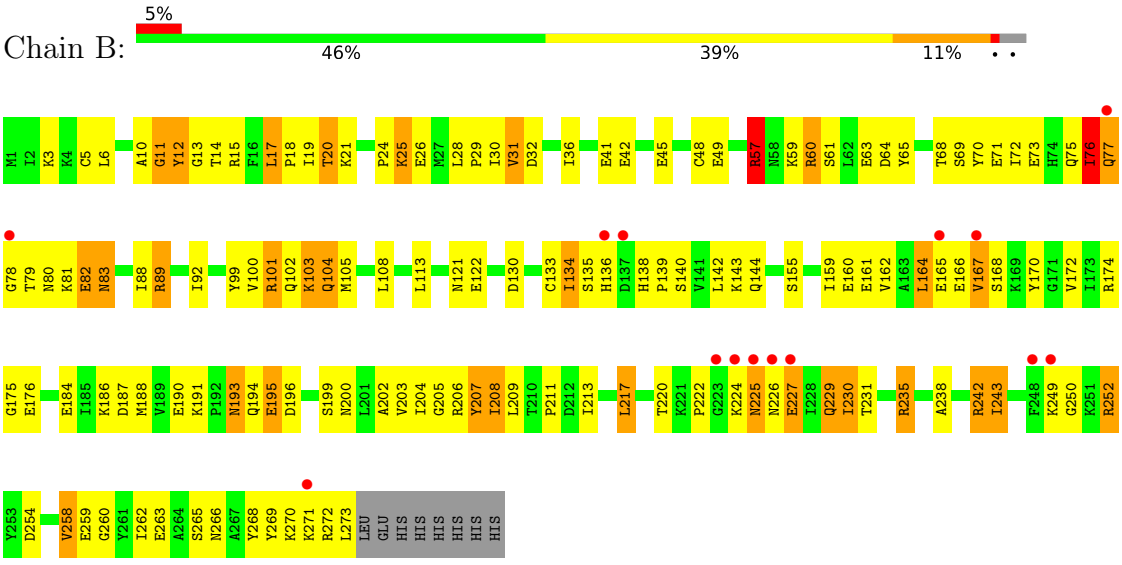
• Molecule 1: UDP-glucose pyrophosphorylase (GalU)

Chain A:



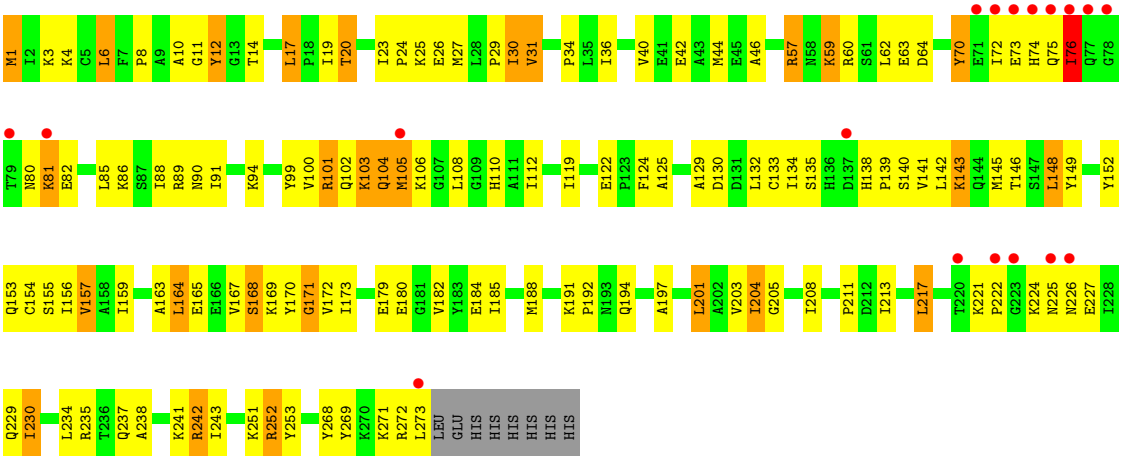
• Molecule 1: UDP-glucose pyrophosphorylase (GalU)

Chain B:



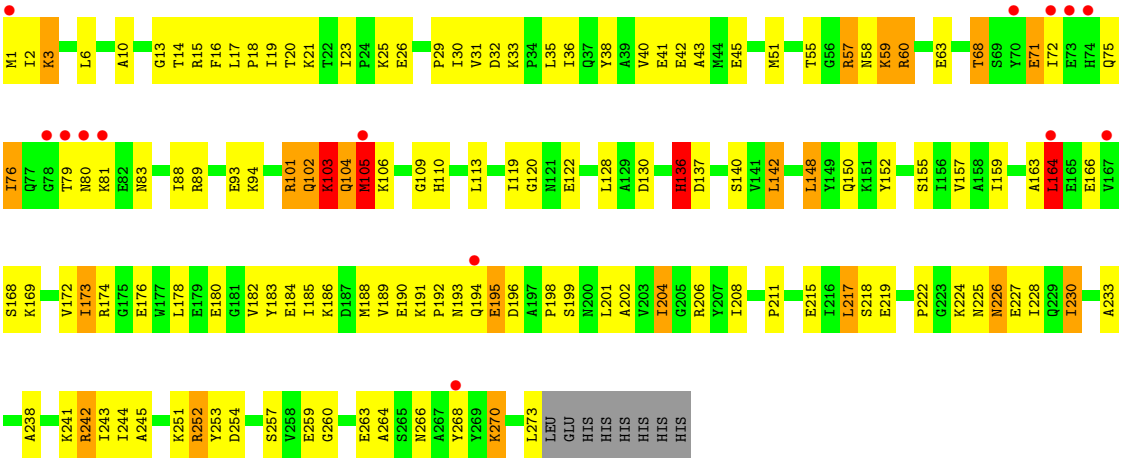
• Molecule 1: UDP-glucose pyrophosphorylase (GalU)

Chain C:



• Molecule 1: UDP-glucose pyrophosphorylase (GalU)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.47Å 98.61Å 245.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.34 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.2 (50.00-2.90) 90.2 (48.34-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.15 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.254 0.225 , 0.254	Depositor DCC
R_{free} test set	2396 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.993	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8783	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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	0.38	0/2210	0.68	1/2978 (0.0%)
1	B	0.40	0/2210	0.69	0/2978
1	C	0.40	0/2210	0.68	2/2978 (0.1%)
1	D	0.39	0/2210	0.68	0/2978
All	All	0.39	0/8840	0.68	3/11912 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	GLY	N-CA-C	-5.47	99.43	113.10
1	C	171	GLY	N-CA-C	-5.03	100.53	113.10
1	C	30	ILE	N-CA-C	-5.01	97.46	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	2172	0	2206	157	0
1	B	2172	0	2206	160	0
1	C	2172	0	2206	144	0
1	D	2172	0	2206	131	0
2	A	20	0	0	1	0
2	B	24	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	2	0
2	D	21	0	0	2	0
All	All	8783	0	8824	555	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 32.

All (555) 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:A:76:ILE:HG23	1:A:82:GLU:HA	1.22	1.10
1:D:76:ILE:HD11	1:D:81:LYS:HB2	1.29	1.10
1:A:79:THR:HG23	1:A:81:LYS:H	1.22	1.04
1:A:179:GLU:HG2	1:A:180:GLU:H	1.23	1.01
1:D:230:ILE:HD12	1:D:230:ILE:H	1.26	1.00
1:A:164:LEU:HD12	1:A:194:GLN:HG3	1.41	0.99
1:C:59:LYS:HE2	1:C:101:ARG:HH21	1.25	0.98
1:D:79:THR:HG22	1:D:80:ASN:H	1.31	0.94
1:A:170:TYR:HE2	1:A:252:ARG:HH22	1.07	0.93
1:B:193:ASN:H	1:B:193:ASN:HD22	1.15	0.93
1:D:104:GLN:O	1:D:106:LYS:HG3	1.67	0.92
1:C:86:LYS:HA	1:C:89:ARG:HH12	1.37	0.90
1:A:242:ARG:HG3	1:A:242:ARG:HH11	1.37	0.90
1:C:17:LEU:HD12	1:C:20:THR:HG22	1.52	0.89
1:C:42:GLU:HG3	1:C:140:SER:HB2	1.54	0.88
1:C:159:ILE:HD12	1:C:201:LEU:HG	1.55	0.88
1:D:204:ILE:HD11	1:D:252:ARG:NH1	1.89	0.88
1:D:224:LYS:HG2	1:D:225:ASN:OD1	1.74	0.87
1:A:19:ILE:HD13	1:B:29:PRO:HB3	1.56	0.87
1:C:19:ILE:HD13	1:D:29:PRO:HB3	1.58	0.85
1:B:161:GLU:HG3	1:B:200:ASN:ND2	1.91	0.85
1:B:176:GLU:HG2	1:B:186:LYS:HE2	1.59	0.84
1:A:103:LYS:HD3	1:A:104:GLN:OE1	1.76	0.84
1:C:12:TYR:HE2	1:C:105:MET:HB2	1.43	0.84
1:B:60:ARG:HG3	1:C:60:ARG:HD3	1.60	0.83
1:C:11:GLY:HA2	1:C:105:MET:HG3	1.60	0.83
1:A:29:PRO:HB3	1:B:19:ILE:HD13	1.60	0.82
1:C:59:LYS:HE2	1:C:101:ARG:NH2	1.94	0.82
1:C:86:LYS:HA	1:C:89:ARG:NH1	1.95	0.81
1:A:270:LYS:O	1:A:273:LEU:HG	1.81	0.81
1:A:79:THR:CG2	1:A:81:LYS:H	1.94	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD21	1:A:242:ARG:NH1	1.97	0.80
1:C:57:ARG:HH21	1:C:57:ARG:HB2	1.46	0.78
1:D:14:THR:HA	1:D:17:LEU:CD2	2.14	0.78
1:C:108:LEU:O	1:C:112:ILE:HG12	1.84	0.78
1:B:213:ILE:HG13	1:B:217:LEU:CD2	2.14	0.77
1:C:81:LYS:HE3	1:C:81:LYS:HA	1.65	0.77
1:A:76:ILE:CG2	1:A:82:GLU:HA	2.11	0.77
1:A:224:LYS:O	1:A:225:ASN:ND2	2.19	0.76
1:D:185:ILE:HD12	1:D:188:MET:HE2	1.68	0.75
1:B:42:GLU:HG3	1:B:140:SER:HB2	1.69	0.75
1:B:193:ASN:H	1:B:193:ASN:ND2	1.85	0.74
1:D:13:GLY:O	1:D:20:THR:HG21	1.86	0.74
1:C:76:ILE:HG23	1:C:76:ILE:O	1.86	0.74
1:A:60:ARG:HH11	1:A:60:ARG:HB3	1.52	0.74
1:A:69:SER:O	1:A:73:GLU:HG3	1.88	0.73
1:A:242:ARG:HG3	1:A:242:ARG:NH1	2.02	0.73
1:B:10:ALA:HB3	1:B:102:GLN:NE2	2.02	0.73
1:A:148:LEU:HD12	1:A:156:ILE:HD13	1.72	0.72
1:A:204:ILE:HD11	1:A:252:ARG:NH1	2.05	0.71
1:D:230:ILE:HD12	1:D:230:ILE:N	2.04	0.71
1:B:238:ALA:HA	1:B:243:ILE:HG23	1.72	0.71
1:C:57:ARG:HB2	1:C:57:ARG:NH2	2.05	0.71
1:A:164:LEU:HD12	1:A:194:GLN:CG	2.21	0.70
1:A:134:ILE:HD13	1:A:135:SER:N	2.07	0.70
1:A:176:GLU:HG3	1:A:186:LYS:HD2	1.73	0.70
1:C:19:ILE:CD1	1:D:29:PRO:HB3	2.21	0.70
1:B:108:LEU:HD23	1:B:230:ILE:HG12	1.73	0.70
1:B:193:ASN:HD22	1:B:193:ASN:N	1.87	0.70
1:C:213:ILE:O	1:C:217:LEU:HD22	1.91	0.70
1:A:179:GLU:HG2	1:A:180:GLU:N	2.04	0.69
1:D:110:HIS:HB2	2:D:282:HOH:O	1.91	0.69
1:D:42:GLU:HG3	1:D:140:SER:HB2	1.74	0.69
1:D:76:ILE:CD1	1:D:81:LYS:HB2	2.15	0.69
1:B:206:ARG:C	1:B:207:TYR:HD1	1.96	0.69
1:B:25:LYS:HE2	1:B:130:ASP:OD1	1.93	0.68
1:B:60:ARG:HH21	1:D:60:ARG:HD3	1.58	0.68
1:A:213:ILE:HG13	1:A:217:LEU:CD2	2.24	0.68
1:B:139:PRO:HB2	1:B:143:LYS:HD3	1.75	0.68
1:D:15:ARG:NH2	1:D:257:SER:HB3	2.09	0.68
1:C:1:MET:HB3	1:C:3:LYS:HE2	1.74	0.68
1:B:31:VAL:HG21	1:B:272:ARG:NH2	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HE2	1:A:110:HIS:CE1	2.29	0.67
1:B:155:SER:HB2	1:B:243:ILE:HB	1.77	0.67
1:C:213:ILE:HG13	1:C:217:LEU:HD22	1.76	0.67
1:A:79:THR:HG23	1:A:81:LYS:N	2.04	0.66
1:D:72:ILE:O	1:D:76:ILE:HB	1.95	0.66
1:C:103:LYS:HE2	1:C:110:HIS:CE1	2.30	0.66
1:B:70:TYR:CE2	1:D:71:GLU:HG3	2.30	0.66
1:B:139:PRO:CB	1:B:143:LYS:HD3	2.26	0.66
1:D:55:THR:HB	1:D:59:LYS:HB3	1.77	0.66
1:B:25:LYS:HD3	1:B:28:LEU:HD12	1.78	0.65
1:B:135:SER:HB2	1:B:138:HIS:HB2	1.79	0.65
1:D:185:ILE:CD1	1:D:245:ALA:HB2	2.27	0.65
1:B:139:PRO:HG2	1:B:144:GLN:HG3	1.79	0.65
1:D:10:ALA:HB3	1:D:105:MET:HE2	1.77	0.65
1:B:225:ASN:HB2	1:B:227:GLU:HG3	1.79	0.65
1:A:127:ILE:HD11	1:A:142:LEU:HG	1.78	0.65
1:D:79:THR:HG22	1:D:80:ASN:N	2.08	0.65
1:C:167:VAL:HG11	1:C:197:ALA:HB2	1.79	0.65
1:D:222:PRO:HB2	1:D:226:ASN:HA	1.79	0.65
1:A:170:TYR:HE2	1:A:252:ARG:NH2	1.89	0.65
1:C:101:ARG:NH1	1:C:101:ARG:HB2	2.12	0.65
1:D:3:LYS:HE3	1:D:3:LYS:HA	1.78	0.64
1:D:119:ILE:HG22	1:D:120:GLY:O	1.96	0.64
1:A:167:VAL:CG1	1:A:192:PRO:HG2	2.28	0.64
1:A:225:ASN:ND2	1:A:225:ASN:O	2.31	0.64
1:A:14:THR:CG2	1:B:81:LYS:HG3	2.28	0.64
1:D:59:LYS:HE2	1:D:101:ARG:HD2	1.79	0.64
1:A:26:GLU:HG3	2:A:294:HOH:O	1.97	0.64
1:B:187:ASP:OD2	1:B:188:MET:N	2.30	0.64
1:A:167:VAL:HG13	1:A:172:VAL:HG21	1.79	0.64
1:B:31:VAL:HG23	1:B:32:ASP:H	1.63	0.63
1:D:169:LYS:HA	1:D:191:LYS:HG2	1.81	0.63
1:A:31:VAL:HG23	1:A:32:ASP:H	1.64	0.63
1:C:213:ILE:HG13	1:C:217:LEU:CD2	2.28	0.63
1:C:273:LEU:O	1:C:273:LEU:HD12	1.98	0.63
1:C:135:SER:OG	1:C:138:HIS:HB2	1.99	0.63
1:C:29:PRO:HB3	1:D:19:ILE:HD13	1.79	0.62
1:D:57:ARG:HA	1:D:57:ARG:CZ	2.29	0.62
1:A:173:ILE:HG23	1:A:174:ARG:N	2.12	0.62
1:A:60:ARG:HD3	1:B:60:ARG:NH2	2.15	0.62
1:A:134:ILE:HB	1:A:268:TYR:OH	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LYS:HD3	1:C:104:GLN:OE1	2.00	0.62
1:B:213:ILE:HG13	1:B:217:LEU:HD22	1.81	0.62
1:B:258:VAL:O	1:B:262:ILE:HG12	2.00	0.62
1:D:176:GLU:OE2	1:D:186:LYS:NZ	2.32	0.62
1:D:195:GLU:CD	1:D:195:GLU:H	2.02	0.62
1:C:14:THR:HG22	1:D:81:LYS:HG2	1.80	0.62
1:A:29:PRO:HB3	1:B:19:ILE:CD1	2.29	0.62
1:B:139:PRO:HB2	1:B:143:LYS:HB3	1.82	0.61
1:B:88:ILE:O	1:B:92:ILE:HG13	2.01	0.61
1:B:79:THR:HG22	1:B:81:LYS:H	1.66	0.61
1:B:81:LYS:C	1:B:83:ASN:H	2.04	0.61
1:B:139:PRO:O	1:B:144:GLN:NE2	2.33	0.61
1:D:189:VAL:O	1:D:189:VAL:HG23	2.01	0.61
1:A:19:ILE:CD1	1:B:29:PRO:HB3	2.28	0.60
1:B:78:GLY:N	1:B:82:GLU:OE1	2.34	0.60
1:A:167:VAL:HG12	1:A:192:PRO:HG2	1.83	0.60
1:C:106:LYS:HD2	1:C:226:ASN:HD21	1.66	0.60
1:D:185:ILE:HD13	1:D:245:ALA:HB2	1.83	0.60
1:D:184:GLU:OE1	1:D:242:ARG:HG3	2.01	0.60
1:A:178:LEU:HD21	1:A:242:ARG:HH12	1.66	0.60
1:C:17:LEU:CD1	1:C:20:THR:HG22	2.30	0.60
1:D:14:THR:HA	1:D:17:LEU:HD23	1.84	0.60
1:C:221:LYS:HG2	2:C:311:HOH:O	2.01	0.60
1:C:106:LYS:O	1:C:227:GLU:HG2	2.01	0.59
1:D:18:PRO:O	1:D:21:LYS:HB3	2.02	0.59
1:D:26:GLU:HB3	1:D:36:ILE:HB	1.83	0.59
1:A:173:ILE:HD11	1:A:188:MET:HE2	1.84	0.59
1:B:89:ARG:HG2	1:B:89:ARG:HH21	1.66	0.59
1:D:183:TYR:HB2	1:D:245:ALA:HB3	1.84	0.59
1:C:188:MET:O	1:C:235:ARG:NH1	2.35	0.59
1:A:80:ASN:H	1:A:80:ASN:ND2	1.99	0.59
1:C:230:ILE:HD12	1:C:230:ILE:N	2.17	0.59
1:B:72:ILE:O	1:B:76:ILE:HB	2.03	0.58
1:C:139:PRO:HB3	1:C:143:LYS:HG2	1.85	0.58
1:D:182:VAL:HG13	1:D:244:ILE:HG23	1.86	0.58
1:B:268:TYR:O	1:B:272:ARG:HG2	2.03	0.58
1:D:230:ILE:H	1:D:230:ILE:CD1	1.98	0.58
1:B:57:ARG:HH21	1:B:105:MET:HE1	1.68	0.58
1:B:164:LEU:HD12	1:B:194:GLN:HA	1.85	0.58
1:D:136:HIS:O	1:D:137:ASP:OD2	2.22	0.58
1:A:4:LYS:HE3	1:A:122:GLU:OE2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HA	1:B:202:ALA:O	2.03	0.58
1:D:168:SER:HA	1:D:192:PRO:O	2.04	0.58
1:D:270:LYS:HD2	1:D:270:LYS:N	2.19	0.58
1:B:42:GLU:HG3	1:B:140:SER:CB	2.33	0.57
1:D:15:ARG:HH21	1:D:257:SER:HB3	1.70	0.57
1:A:76:ILE:HG23	1:A:82:GLU:CA	2.16	0.57
1:B:134:ILE:HD13	1:B:135:SER:N	2.19	0.57
1:D:102:GLN:HE21	1:D:105:MET:HE2	1.69	0.57
1:C:30:ILE:HG22	1:C:31:VAL:HG22	1.86	0.57
1:A:57:ARG:HG2	1:B:71:GLU:OE1	2.05	0.57
1:A:230:ILE:HD12	1:A:231:THR:H	1.69	0.57
1:C:155:SER:HA	1:C:208:ILE:O	2.04	0.57
1:C:70:TYR:HA	1:C:73:GLU:HB3	1.87	0.57
1:A:176:GLU:OE2	1:A:186:LYS:HD2	2.05	0.57
1:B:184:GLU:OE1	1:B:242:ARG:NH1	2.37	0.57
1:C:179:GLU:HG2	1:C:182:VAL:HB	1.87	0.57
1:B:60:ARG:HD2	1:B:64:ASP:OD2	2.04	0.57
1:C:34:PRO:HG3	1:D:19:ILE:HG13	1.86	0.56
1:A:186:LYS:HE2	1:A:186:LYS:HA	1.87	0.56
1:C:59:LYS:HD2	1:C:60:ARG:N	2.20	0.56
1:A:76:ILE:HD12	1:A:81:LYS:O	2.06	0.56
1:B:30:ILE:HG22	1:B:31:VAL:N	2.20	0.56
1:C:30:ILE:HG22	1:C:31:VAL:N	2.20	0.56
1:D:104:GLN:O	1:D:106:LYS:HE3	2.06	0.56
1:D:264:ALA:O	1:D:268:TYR:HD2	1.89	0.56
1:C:72:ILE:O	1:C:72:ILE:HG12	2.04	0.56
1:C:85:LEU:HD21	1:D:17:LEU:HD12	1.86	0.56
1:B:160:GLU:OE2	1:B:252:ARG:HD2	2.06	0.56
1:D:155:SER:HA	1:D:208:ILE:O	2.06	0.56
1:D:174:ARG:HG3	1:D:198:PRO:HB2	1.87	0.56
1:D:244:ILE:HG22	1:D:245:ALA:N	2.21	0.56
1:B:69:SER:O	1:B:73:GLU:HG3	2.05	0.56
1:D:204:ILE:HD11	1:D:252:ARG:HH11	1.70	0.56
1:B:167:VAL:HG22	1:B:172:VAL:HG21	1.87	0.56
1:A:180:GLU:O	1:A:182:VAL:HG23	2.06	0.56
1:C:12:TYR:CE2	1:C:105:MET:HB2	2.32	0.55
1:D:1:MET:HB2	1:D:3:LYS:NZ	2.20	0.55
1:D:225:ASN:O	1:D:226:ASN:C	2.45	0.55
1:B:63:GLU:HG2	1:B:99:TYR:CE2	2.40	0.55
1:C:134:ILE:HD12	1:C:271:LYS:HE2	1.88	0.55
1:D:102:GLN:HE21	1:D:105:MET:CE	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HG23	1:A:244:ILE:HG22	1.88	0.55
1:D:254:ASP:O	1:D:260:GLY:HA3	2.06	0.55
1:C:29:PRO:HB3	1:D:19:ILE:CD1	2.36	0.55
1:B:187:ASP:OD2	1:B:235:ARG:HD3	2.07	0.55
1:B:190:GLU:HG2	1:B:224:LYS:NZ	2.21	0.55
1:A:119:ILE:HD12	1:A:119:ILE:N	2.21	0.55
1:A:26:GLU:H	1:A:26:GLU:CD	2.10	0.55
1:C:204:ILE:CG2	1:C:205:GLY:N	2.69	0.55
1:B:70:TYR:HE2	1:D:71:GLU:HG3	1.70	0.54
1:B:204:ILE:HG22	1:B:205:GLY:N	2.23	0.54
1:B:230:ILE:HD12	1:B:231:THR:H	1.72	0.54
1:C:142:LEU:HD13	1:C:146:THR:HG23	1.89	0.54
1:A:14:THR:HA	1:A:17:LEU:CD2	2.38	0.54
1:C:57:ARG:HD2	1:D:71:GLU:OE1	2.08	0.54
1:C:148:LEU:HD22	1:C:152:TYR:HD2	1.73	0.54
1:A:185:ILE:HD13	1:A:188:MET:HE2	1.89	0.54
1:B:57:ARG:HH11	1:B:101:ARG:NH2	2.04	0.54
1:D:31:VAL:CG2	1:D:32:ASP:N	2.70	0.54
1:D:173:ILE:HG23	1:D:174:ARG:N	2.22	0.54
1:D:215:GLU:O	1:D:218:SER:HB3	2.08	0.54
1:A:159:ILE:HD12	1:A:201:LEU:HG	1.89	0.54
1:A:230:ILE:HD12	1:A:231:THR:N	2.23	0.53
1:B:3:LYS:HE3	1:B:49:GLU:OE2	2.08	0.53
1:C:101:ARG:HB2	1:C:101:ARG:HH11	1.71	0.53
1:B:11:GLY:O	1:B:13:GLY:N	2.41	0.53
1:B:188:MET:HE1	1:B:203:VAL:HG21	1.90	0.53
1:D:122:GLU:C	1:D:211:PRO:HG3	2.28	0.53
1:A:31:VAL:HG21	1:A:272:ARG:HH12	1.71	0.53
1:A:108:LEU:HD23	1:A:230:ILE:HG12	1.90	0.53
1:D:193:ASN:HB2	1:D:196:ASP:OD2	2.08	0.53
1:A:60:ARG:HB3	1:A:60:ARG:NH1	2.21	0.53
1:A:72:ILE:HG12	1:A:72:ILE:O	2.09	0.53
1:A:166:GLU:OE2	1:A:169:LYS:HE2	2.08	0.53
1:C:88:ILE:HG23	1:C:89:ARG:N	2.24	0.53
1:D:217:LEU:HD13	1:D:233:ALA:HB2	1.91	0.53
1:C:104:GLN:HB2	1:C:106:LYS:HZ2	1.74	0.53
1:D:57:ARG:HA	1:D:57:ARG:NH2	2.24	0.53
1:A:80:ASN:C	1:A:81:LYS:HE3	2.30	0.53
1:D:60:ARG:NH2	1:D:63:GLU:OE1	2.42	0.53
1:D:238:ALA:HB2	1:D:243:ILE:HD11	1.90	0.53
1:A:30:ILE:HG22	1:A:31:VAL:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:HG13	1:B:217:LEU:HD21	1.90	0.53
1:B:81:LYS:O	1:B:83:ASN:N	2.43	0.52
1:B:164:LEU:HD12	1:B:194:GLN:CB	2.40	0.52
1:D:148:LEU:HD22	1:D:152:TYR:CD2	2.45	0.52
1:A:173:ILE:CG2	1:A:174:ARG:N	2.73	0.52
1:C:204:ILE:HG23	1:C:205:GLY:N	2.24	0.52
1:B:10:ALA:HB3	1:B:102:GLN:HE21	1.71	0.52
1:C:157:VAL:HG23	1:C:203:VAL:HG13	1.92	0.52
1:D:33:LYS:HE2	1:D:38:TYR:CZ	2.45	0.52
1:B:188:MET:CE	1:B:203:VAL:HG21	2.40	0.52
1:A:6:LEU:HD21	1:A:54:VAL:HG23	1.90	0.52
1:B:134:ILE:HD13	1:B:135:SER:H	1.75	0.52
1:C:132:LEU:HD21	1:C:268:TYR:CE2	2.45	0.52
1:D:206:ARG:HG2	1:D:206:ARG:HH11	1.75	0.52
1:A:103:LYS:H	1:A:103:LYS:HD2	1.75	0.51
1:A:186:LYS:O	1:A:187:ASP:HB2	2.11	0.51
1:C:46:ALA:CB	1:C:142:LEU:HD12	2.41	0.51
1:B:164:LEU:HD12	1:B:194:GLN:HG2	1.93	0.51
1:C:108:LEU:HD23	1:C:230:ILE:HG12	1.92	0.51
1:D:104:GLN:O	1:D:106:LYS:CG	2.52	0.51
1:C:237:GLN:HG2	1:C:243:ILE:HG21	1.93	0.51
1:A:148:LEU:CD1	1:A:156:ILE:HD13	2.40	0.51
1:A:180:GLU:HA	1:A:180:GLU:OE1	2.11	0.51
1:D:222:PRO:HB2	1:D:226:ASN:CA	2.40	0.51
1:A:30:ILE:HG22	1:A:31:VAL:HG22	1.93	0.51
1:C:1:MET:HB3	1:C:3:LYS:CE	2.39	0.51
1:D:43:ALA:HA	1:D:142:LEU:HD12	1.92	0.51
1:D:1:MET:HB2	1:D:3:LYS:HZ2	1.75	0.51
1:A:119:ILE:HG21	1:A:124:PHE:CD2	2.45	0.51
1:D:164:LEU:HD12	1:D:194:GLN:NE2	2.26	0.50
1:A:103:LYS:HD2	1:A:103:LYS:N	2.26	0.50
1:B:225:ASN:CB	1:B:227:GLU:HG3	2.41	0.50
1:C:59:LYS:HD2	1:C:60:ARG:H	1.75	0.50
1:D:41:GLU:HG3	1:D:45:GLU:OE2	2.12	0.50
1:A:158:ALA:HB3	1:A:206:ARG:HB2	1.94	0.50
1:B:204:ILE:CG2	1:B:205:GLY:N	2.74	0.50
1:C:59:LYS:HG2	1:C:101:ARG:CZ	2.42	0.50
1:C:167:VAL:C	1:C:169:LYS:H	2.15	0.50
1:D:174:ARG:CG	1:D:198:PRO:HB2	2.42	0.50
1:B:77:GLN:HG3	1:B:82:GLU:OE1	2.12	0.50
1:B:164:LEU:HD12	1:B:194:GLN:CA	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ILE:O	1:C:40:VAL:HG23	2.12	0.50
1:C:149:TYR:O	1:C:153:GLN:NE2	2.45	0.50
1:B:17:LEU:HD13	1:B:20:THR:HG22	1.93	0.50
1:C:76:ILE:O	1:C:76:ILE:CG2	2.58	0.50
1:A:6:LEU:CD2	1:A:54:VAL:HG23	2.42	0.49
1:A:55:THR:HB	1:A:59:LYS:HB3	1.93	0.49
1:A:128:LEU:HD23	1:A:128:LEU:N	2.27	0.49
1:B:207:TYR:N	1:B:207:TYR:CD1	2.79	0.49
1:B:238:ALA:CA	1:B:243:ILE:HG23	2.42	0.49
1:A:166:GLU:OE2	1:A:169:LYS:CE	2.60	0.49
1:C:23:ILE:HD12	1:D:23:ILE:HD12	1.94	0.49
1:A:3:LYS:HE3	1:A:3:LYS:HA	1.93	0.49
1:A:113:LEU:HG	1:A:217:LEU:HB3	1.93	0.49
1:A:17:LEU:HD13	1:A:20:THR:HG22	1.95	0.49
1:B:161:GLU:HG3	1:B:200:ASN:HD21	1.73	0.49
1:D:159:ILE:HA	1:D:202:ALA:O	2.13	0.49
1:D:215:GLU:OE2	1:D:219:GLU:OE1	2.31	0.49
1:B:57:ARG:NH2	1:B:105:MET:HE1	2.28	0.49
1:B:138:HIS:CE1	1:B:249:LYS:HD3	2.47	0.49
1:B:230:ILE:HD12	1:B:230:ILE:N	2.26	0.49
1:D:204:ILE:CG1	1:D:252:ARG:HD2	2.43	0.49
1:A:80:ASN:ND2	1:A:81:LYS:NZ	2.60	0.49
1:A:142:LEU:HD13	1:A:142:LEU:O	2.13	0.49
1:C:20:THR:O	1:C:20:THR:HG23	2.13	0.49
1:C:80:ASN:ND2	1:C:81:LYS:NZ	2.60	0.49
1:A:225:ASN:O	1:A:225:ASN:CG	2.51	0.48
1:B:193:ASN:ND2	1:B:196:ASP:OD2	2.45	0.48
1:D:273:LEU:HD12	1:D:273:LEU:C	2.33	0.48
1:B:133:CYS:SG	1:B:252:ARG:HB2	2.53	0.48
1:B:170:TYR:O	1:B:191:LYS:HA	2.12	0.48
1:C:81:LYS:HE3	1:C:81:LYS:CA	2.39	0.48
1:C:106:LYS:C	1:C:227:GLU:HG2	2.34	0.48
1:D:148:LEU:HD22	1:D:152:TYR:HD2	1.78	0.48
1:B:266:ASN:O	1:B:270:LYS:HG3	2.13	0.48
1:C:106:LYS:CD	1:C:226:ASN:HD21	2.26	0.48
1:C:171:GLY:O	1:C:203:VAL:HG23	2.13	0.48
1:D:251:LYS:HE3	1:D:253:TYR:CE2	2.47	0.48
1:A:1:MET:CB	1:A:3:LYS:HZ2	2.26	0.48
1:A:193:ASN:HB2	1:A:196:ASP:OD2	2.14	0.48
1:C:89:ARG:CZ	1:C:89:ARG:HB3	2.43	0.48
1:D:16:PHE:CE1	1:D:25:LYS:HE3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HG3	1:A:140:SER:HB2	1.95	0.48
1:A:81:LYS:HG2	1:B:14:THR:HG22	1.93	0.48
1:A:84:ALA:HB1	1:B:17:LEU:HB3	1.96	0.48
1:B:122:GLU:O	1:B:211:PRO:HG3	2.13	0.48
1:A:1:MET:CB	1:A:3:LYS:NZ	2.77	0.48
1:A:6:LEU:HD21	1:A:54:VAL:CG2	2.44	0.48
1:B:26:GLU:HB3	1:B:36:ILE:HB	1.96	0.48
1:C:273:LEU:O	1:C:273:LEU:CD1	2.62	0.48
1:B:100:VAL:O	1:B:100:VAL:HG13	2.14	0.48
1:B:259:GLU:O	1:B:263:GLU:HG3	2.13	0.48
1:D:106:LYS:HB2	2:D:282:HOH:O	2.13	0.48
1:C:63:GLU:HG2	1:C:99:TYR:CE2	2.49	0.47
1:C:134:ILE:CD1	1:C:271:LYS:HE2	2.44	0.47
1:B:18:PRO:O	1:B:21:LYS:HB3	2.14	0.47
1:B:136:HIS:CE1	1:B:250:GLY:HA2	2.50	0.47
1:C:204:ILE:HG23	1:C:205:GLY:H	1.79	0.47
1:B:164:LEU:CD1	1:B:194:GLN:HA	2.44	0.47
1:B:222:PRO:HB3	1:B:226:ASN:C	2.35	0.47
1:D:60:ARG:NE	1:D:60:ARG:HA	2.29	0.47
1:A:81:LYS:C	1:A:83:ASN:H	2.18	0.47
1:A:266:ASN:O	1:A:270:LYS:HD3	2.14	0.47
1:B:170:TYR:HE2	1:B:252:ARG:HH22	1.61	0.47
1:C:103:LYS:HD3	1:C:104:GLN:CD	2.35	0.47
1:A:160:GLU:OE2	1:A:252:ARG:HD2	2.14	0.47
1:C:103:LYS:HE2	1:C:110:HIS:HE1	1.78	0.47
1:C:44:MET:CE	1:C:91:ILE:HG12	2.44	0.47
1:C:81:LYS:HA	1:C:81:LYS:CE	2.38	0.47
1:A:246:TYR:CE2	1:A:248:PHE:HA	2.50	0.47
1:C:10:ALA:CB	1:C:102:GLN:NE2	2.78	0.47
1:C:125:ALA:HB1	1:C:142:LEU:HD21	1.97	0.47
1:D:57:ARG:HG3	1:D:58:ASN:ND2	2.30	0.47
1:A:259:GLU:O	1:A:263:GLU:HG3	2.14	0.47
1:C:164:LEU:HD11	1:C:194:GLN:NE2	2.29	0.47
1:B:25:LYS:HD2	1:B:25:LYS:O	2.15	0.47
1:B:207:TYR:HD1	1:B:207:TYR:N	2.13	0.47
1:D:102:GLN:O	1:D:103:LYS:O	2.33	0.47
1:A:71:GLU:HG2	1:B:57:ARG:HD3	1.97	0.47
1:A:57:ARG:NH2	1:D:68:THR:CG2	2.78	0.46
1:A:164:LEU:HB3	1:A:194:GLN:HE21	1.80	0.46
1:C:134:ILE:HB	1:C:268:TYR:OH	2.14	0.46
1:C:167:VAL:HG13	1:C:192:PRO:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:THR:O	1:D:17:LEU:HD23	2.15	0.46
1:A:6:LEU:HG	1:A:119:ILE:HD11	1.97	0.46
1:A:30:ILE:HD13	1:A:30:ILE:HA	1.74	0.46
1:A:79:THR:O	1:A:82:GLU:HG2	2.15	0.46
1:B:164:LEU:O	1:B:194:GLN:HG2	2.14	0.46
1:D:185:ILE:HD11	1:D:245:ALA:HB2	1.96	0.46
1:B:174:ARG:O	1:B:186:LYS:HB2	2.15	0.46
1:B:162:VAL:HB	1:B:166:GLU:HG3	1.98	0.46
1:B:206:ARG:HG2	1:B:206:ARG:HH11	1.80	0.46
1:D:40:VAL:HG13	1:D:51:MET:HE3	1.98	0.46
1:A:122:GLU:C	1:A:211:PRO:HG3	2.36	0.46
1:B:79:THR:HG22	1:B:80:ASN:N	2.29	0.46
1:A:167:VAL:O	1:A:169:LYS:N	2.49	0.46
1:B:10:ALA:CB	1:B:102:GLN:HE21	2.29	0.46
1:B:224:LYS:O	1:B:225:ASN:CG	2.54	0.46
1:A:1:MET:HB3	1:A:3:LYS:NZ	2.31	0.46
1:C:122:GLU:C	1:C:211:PRO:HG3	2.35	0.46
1:D:178:LEU:HD21	1:D:242:ARG:NH2	2.30	0.46
1:A:212:ASP:OD2	1:A:237:GLN:NE2	2.49	0.46
1:C:26:GLU:CD	1:C:26:GLU:H	2.20	0.46
1:C:122:GLU:CA	1:C:211:PRO:HG3	2.46	0.46
1:D:17:LEU:HD13	1:D:20:THR:HG22	1.98	0.46
1:A:13:GLY:O	1:A:20:THR:HG21	2.16	0.46
1:A:167:VAL:HG11	1:A:197:ALA:CB	2.45	0.46
1:B:30:ILE:HD13	1:B:30:ILE:HA	1.72	0.46
1:C:60:ARG:HD2	1:C:64:ASP:OD1	2.16	0.46
1:D:173:ILE:CG2	1:D:174:ARG:N	2.79	0.46
1:A:1:MET:HB2	1:A:3:LYS:HZ2	1.81	0.45
1:D:190:GLU:O	1:D:191:LYS:C	2.54	0.45
1:A:29:PRO:HG3	1:B:28:LEU:HD22	1.98	0.45
1:A:216:ILE:CD1	1:A:237:GLN:HG2	2.46	0.45
1:C:59:LYS:O	1:C:60:ARG:C	2.55	0.45
1:C:85:LEU:HD23	1:D:18:PRO:HB3	1.97	0.45
1:A:103:LYS:HE2	1:A:110:HIS:NE2	2.30	0.45
1:A:225:ASN:O	1:A:227:GLU:N	2.50	0.45
1:C:184:GLU:OE1	1:C:242:ARG:NH1	2.49	0.45
1:B:229:GLN:HE21	1:B:229:GLN:HB3	1.63	0.45
1:A:15:ARG:CZ	1:A:256:GLY:O	2.65	0.45
1:A:24:PRO:HG2	1:A:27:MET:HB2	1.98	0.45
1:A:172:VAL:HG11	1:A:199:SER:O	2.17	0.45
1:B:60:ARG:O	1:B:64:ASP:CG	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LYS:HG2	1:D:14:THR:O	2.16	0.45
1:B:12:TYR:O	1:B:20:THR:HG21	2.17	0.45
1:C:133:CYS:SG	1:C:252:ARG:HB2	2.56	0.45
1:D:185:ILE:HG13	1:D:243:ILE:HG13	1.99	0.45
1:A:74:HIS:O	1:A:75:GLN:C	2.54	0.45
1:B:57:ARG:O	1:B:101:ARG:NH1	2.49	0.45
1:D:17:LEU:HD22	1:D:20:THR:CG2	2.46	0.45
1:C:119:ILE:HG21	1:C:124:PHE:CD2	2.52	0.45
1:C:251:LYS:HE3	1:C:253:TYR:CZ	2.52	0.45
1:D:109:GLY:HA3	1:D:228:ILE:HB	1.99	0.45
1:D:198:PRO:O	1:D:199:SER:HB3	2.16	0.45
1:C:25:LYS:HZ3	1:C:130:ASP:CG	2.17	0.45
1:D:152:TYR:CD1	1:D:244:ILE:HD11	2.52	0.45
1:C:230:ILE:N	1:C:230:ILE:CD1	2.79	0.44
1:C:230:ILE:O	1:C:234:LEU:HG	2.17	0.44
1:A:209:LEU:HD13	1:A:213:ILE:HG12	2.00	0.44
1:C:60:ARG:O	1:C:64:ASP:OD1	2.35	0.44
1:C:173:ILE:CD1	1:C:188:MET:HG2	2.47	0.44
1:C:192:PRO:HG2	1:C:197:ALA:HB2	2.00	0.44
1:B:12:TYR:O	1:B:13:GLY:C	2.56	0.44
1:B:25:LYS:HD2	1:B:25:LYS:C	2.37	0.44
1:B:103:LYS:HB2	1:B:104:GLN:OE1	2.18	0.44
1:C:59:LYS:HD3	1:C:63:GLU:OE2	2.18	0.44
1:D:266:ASN:O	1:D:270:LYS:HD3	2.18	0.44
1:B:68:THR:HG1	1:B:70:TYR:HE1	1.64	0.44
1:C:24:PRO:HG2	1:C:27:MET:HG2	1.99	0.44
1:C:30:ILE:HG22	1:C:31:VAL:CG2	2.47	0.44
1:A:259:GLU:HG3	1:B:269:TYR:OH	2.17	0.44
1:B:57:ARG:NH1	1:B:101:ARG:NH2	2.66	0.44
1:D:59:LYS:O	1:D:63:GLU:HG3	2.18	0.44
1:D:102:GLN:C	1:D:103:LYS:O	2.54	0.44
1:D:244:ILE:CG2	1:D:245:ALA:N	2.80	0.44
1:C:11:GLY:N	1:C:105:MET:HE2	2.33	0.44
1:C:164:LEU:HD13	1:C:164:LEU:C	2.38	0.44
1:D:189:VAL:O	1:D:192:PRO:HD3	2.17	0.44
1:B:5:CYS:HB2	1:B:48:CYS:SG	2.58	0.44
1:B:41:GLU:O	1:B:45:GLU:HG3	2.18	0.43
1:C:20:THR:HA	1:C:23:ILE:O	2.17	0.43
1:A:174:ARG:HG3	1:A:198:PRO:HB2	2.00	0.43
1:B:24:PRO:HA	2:B:297:HOH:O	2.17	0.43
1:C:12:TYR:N	1:C:12:TYR:CD2	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ALA:HB3	1:C:142:LEU:HD12	2.00	0.43
1:C:59:LYS:HG2	1:C:101:ARG:NH2	2.33	0.43
1:A:254:ASP:C	1:A:256:GLY:H	2.20	0.43
1:A:169:LYS:HG3	1:A:170:TYR:CE1	2.53	0.43
1:B:10:ALA:CB	1:B:105:MET:HG3	2.48	0.43
1:C:24:PRO:HG2	1:C:27:MET:CG	2.49	0.43
1:D:30:ILE:HD13	1:D:30:ILE:HA	1.78	0.43
1:D:184:GLU:HG2	1:D:186:LYS:HE3	2.01	0.43
1:B:160:GLU:N	1:B:202:ALA:O	2.47	0.43
1:A:17:LEU:HD11	1:B:72:ILE:CD1	2.48	0.43
1:A:17:LEU:HD11	1:B:72:ILE:HD13	2.01	0.43
1:B:172:VAL:HG11	1:B:199:SER:O	2.18	0.43
1:C:104:GLN:OE1	1:C:104:GLN:O	2.36	0.43
1:B:10:ALA:O	1:B:11:GLY:C	2.57	0.43
1:B:57:ARG:HA	1:B:57:ARG:NE	2.34	0.43
1:D:164:LEU:HD12	1:D:194:GLN:HE21	1.84	0.43
1:A:80:ASN:ND2	1:A:80:ASN:N	2.62	0.43
1:A:155:SER:HA	1:A:208:ILE:O	2.19	0.43
1:B:217:LEU:O	1:B:220:THR:HB	2.18	0.43
1:D:163:ALA:O	1:D:166:GLU:N	2.52	0.43
1:A:20:THR:HG23	1:A:20:THR:O	2.18	0.43
1:B:60:ARG:HG3	1:C:60:ARG:CD	2.39	0.43
1:B:105:MET:SD	1:B:105:MET:N	2.92	0.43
1:C:167:VAL:O	1:C:169:LYS:N	2.51	0.43
1:C:229:GLN:NE2	1:C:229:GLN:HA	2.34	0.43
1:A:176:GLU:CG	1:A:186:LYS:HD2	2.45	0.42
1:B:139:PRO:HB3	1:B:143:LYS:HD3	1.99	0.42
1:C:272:ARG:HD3	1:C:272:ARG:HA	1.84	0.42
1:B:70:TYR:CD2	1:D:71:GLU:HG3	2.54	0.42
1:B:155:SER:HA	1:B:208:ILE:O	2.19	0.42
1:B:222:PRO:HA	1:B:227:GLU:O	2.19	0.42
1:C:225:ASN:O	1:C:226:ASN:HB3	2.18	0.42
1:D:186:LYS:HA	1:D:186:LYS:HD3	1.82	0.42
1:A:204:ILE:HD12	1:A:204:ILE:HA	1.77	0.42
1:C:269:TYR:O	1:C:272:ARG:HB2	2.20	0.42
1:B:138:HIS:ND1	1:B:249:LYS:HB3	2.34	0.42
1:B:273:LEU:HD12	1:B:273:LEU:C	2.40	0.42
1:C:104:GLN:HB2	1:C:106:LYS:NZ	2.34	0.42
1:A:33:LYS:HA	1:B:19:ILE:HB	2.01	0.42
1:A:166:GLU:O	1:A:169:LYS:HG2	2.19	0.42
1:A:139:PRO:HG2	1:A:144:GLN:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:H	1:B:166:GLU:HG2	1.66	0.42
1:B:209:LEU:HD13	1:B:213:ILE:HG12	2.01	0.42
1:C:90:ASN:O	1:C:94:LYS:HB2	2.19	0.42
1:C:141:VAL:O	1:C:145:MET:HG3	2.19	0.42
1:C:170:TYR:O	1:C:191:LYS:N	2.52	0.42
1:D:59:LYS:HE2	1:D:101:ARG:CD	2.47	0.42
1:D:273:LEU:HD12	1:D:273:LEU:O	2.19	0.42
1:A:115:GLY:O	1:A:119:ILE:HD13	2.20	0.42
1:A:229:GLN:O	1:A:231:THR:N	2.53	0.42
1:B:121:ASN:OD1	1:B:121:ASN:O	2.37	0.42
1:B:235:ARG:HH11	1:B:235:ARG:HG3	1.85	0.42
1:C:238:ALA:HB2	1:C:243:ILE:HD11	2.02	0.42
1:B:81:LYS:C	1:B:83:ASN:N	2.69	0.42
1:C:167:VAL:HG12	1:C:168:SER:N	2.34	0.42
1:C:60:ARG:HB3	2:C:309:HOH:O	2.18	0.41
1:C:101:ARG:HH11	1:C:101:ARG:CB	2.33	0.41
1:D:93:GLU:HG2	1:D:94:LYS:N	2.35	0.41
1:A:76:ILE:O	1:A:79:THR:HB	2.20	0.41
1:A:273:LEU:O	1:A:273:LEU:CD1	2.68	0.41
1:C:4:LYS:HD3	1:C:119:ILE:HA	2.02	0.41
1:D:93:GLU:HG2	1:D:94:LYS:HG3	2.02	0.41
1:A:14:THR:HG21	1:B:81:LYS:HG3	2.00	0.41
1:A:42:GLU:OE2	1:A:206:ARG:NE	2.47	0.41
1:A:242:ARG:HH11	1:A:242:ARG:CG	2.16	0.41
1:D:172:VAL:CG1	1:D:173:ILE:N	2.83	0.41
1:A:1:MET:HB2	1:A:3:LYS:NZ	2.36	0.41
1:A:157:VAL:O	1:A:157:VAL:HG22	2.20	0.41
1:B:31:VAL:HG23	1:B:32:ASP:N	2.32	0.41
1:B:176:GLU:HG2	1:B:186:LYS:CE	2.40	0.41
1:C:11:GLY:CA	1:C:105:MET:HG3	2.42	0.41
1:A:167:VAL:HG11	1:A:197:ALA:HB2	2.02	0.41
1:A:193:ASN:HB2	1:A:196:ASP:CG	2.41	0.41
1:B:164:LEU:O	1:B:167:VAL:HB	2.21	0.41
1:D:17:LEU:HA	1:D:20:THR:HG22	2.03	0.41
1:B:122:GLU:N	1:B:211:PRO:CG	2.83	0.41
1:B:175:GLY:HA2	1:B:186:LYS:HG2	2.01	0.41
1:C:154:CYS:O	1:C:156:ILE:HG13	2.21	0.41
1:D:204:ILE:HG12	1:D:252:ARG:HD2	2.02	0.41
1:A:21:LYS:NZ	1:B:65:TYR:O	2.53	0.41
1:A:164:LEU:HB3	1:A:194:GLN:NE2	2.36	0.41
1:B:254:ASP:O	1:B:260:GLY:HA3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLU:N	1:C:211:PRO:HG3	2.36	0.41
1:B:57:ARG:HH11	1:B:101:ARG:HH22	1.69	0.41
1:C:6:LEU:O	1:C:8:PRO:HD3	2.21	0.41
1:C:19:ILE:HB	1:D:32:ASP:O	2.20	0.41
1:D:10:ALA:CB	1:D:102:GLN:HG3	2.51	0.41
1:A:32:ASP:HB2	1:B:17:LEU:O	2.20	0.41
1:A:103:LYS:H	1:A:103:LYS:CD	2.29	0.41
1:B:10:ALA:CB	1:B:102:GLN:NE2	2.78	0.41
1:B:168:SER:O	1:B:191:LYS:HG2	2.20	0.41
1:B:193:ASN:OD1	1:B:195:GLU:HG2	2.20	0.41
1:C:4:LYS:CD	1:C:119:ILE:HA	2.51	0.41
1:C:26:GLU:HB3	1:C:36:ILE:HB	2.02	0.41
1:C:163:ALA:O	1:C:165:GLU:N	2.54	0.41
1:A:81:LYS:N	1:A:81:LYS:HE3	2.36	0.41
1:A:204:ILE:HG23	1:A:205:GLY:N	2.36	0.41
1:A:223:GLY:O	1:A:225:ASN:N	2.54	0.41
1:B:60:ARG:O	1:B:64:ASP:CB	2.69	0.41
1:B:213:ILE:O	1:B:217:LEU:HD22	2.20	0.41
1:C:167:VAL:HG22	1:C:172:VAL:HG21	2.02	0.41
1:A:80:ASN:HD22	1:A:81:LYS:HE3	1.86	0.40
1:A:139:PRO:HG2	1:A:144:GLN:CG	2.51	0.40
1:C:100:VAL:O	1:C:100:VAL:HG13	2.21	0.40
1:D:3:LYS:HE3	1:D:3:LYS:CA	2.47	0.40
1:B:70:TYR:O	1:B:71:GLU:C	2.59	0.40
1:C:10:ALA:HB3	1:C:105:MET:CE	2.51	0.40
1:A:20:THR:O	1:A:20:THR:CG2	2.68	0.40
1:A:217:LEU:HD13	1:A:217:LEU:HA	1.91	0.40
1:C:157:VAL:HG13	1:C:185:ILE:HD11	2.04	0.40
1:D:88:ILE:HG23	1:D:89:ARG:N	2.35	0.40
1:A:10:ALA:CB	1:A:102:GLN:NE2	2.85	0.40
1:A:162:VAL:O	1:A:200:ASN:HB2	2.22	0.40
1:D:259:GLU:HG2	1:D:263:GLU:OE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/281 (96%)	233 (86%)	31 (11%)	7 (3%)	5	20
1	B	271/281 (96%)	233 (86%)	30 (11%)	8 (3%)	4	17
1	C	271/281 (96%)	235 (87%)	27 (10%)	9 (3%)	4	15
1	D	271/281 (96%)	235 (87%)	27 (10%)	9 (3%)	4	15
All	All	1084/1124 (96%)	936 (86%)	115 (11%)	33 (3%)	4	17

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	B	12	TYR
1	B	57	ARG
1	B	76	ILE
1	C	75	GLN
1	C	164	LEU
1	C	222	PRO
1	A	136	HIS
1	A	168	SER
1	A	224	LYS
1	A	226	ASN
1	A	230	ILE
1	B	82	GLU
1	B	208	ILE
1	B	225	ASN
1	C	168	SER
1	C	224	LYS
1	D	103	LYS
1	D	104	GLN
1	D	226	ASN
1	C	76	ILE
1	C	129	ALA
1	D	105	MET
1	D	136	HIS
1	C	82	GLU
1	C	180	GLU
1	D	71	GLU
1	D	180	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	GLU
1	B	271	LYS
1	D	164	LEU
1	B	11	GLY
1	D	2	ILE

5.3.2 Protein sidechains (i)

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	236/244 (97%)	200 (85%)	36 (15%)	2 8
1	B	236/244 (97%)	199 (84%)	37 (16%)	2 8
1	C	236/244 (97%)	209 (89%)	27 (11%)	5 17
1	D	236/244 (97%)	202 (86%)	34 (14%)	3 9
All	All	944/976 (97%)	810 (86%)	134 (14%)	3 10

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6	LEU
1	A	20	THR
1	A	31	VAL
1	A	32	ASP
1	A	35	LEU
1	A	59	LYS
1	A	60	ARG
1	A	62	LEU
1	A	67	ASP
1	A	79	THR
1	A	80	ASN
1	A	81	LYS
1	A	90	ASN
1	A	103	LYS
1	A	104	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	105	MET
1	A	128	LEU
1	A	134	ILE
1	A	138	HIS
1	A	157	VAL
1	A	164	LEU
1	A	173	ILE
1	A	189	VAL
1	A	196	ASP
1	A	201	LEU
1	A	204	ILE
1	A	217	LEU
1	A	225	ASN
1	A	229	GLN
1	A	230	ILE
1	A	241	LYS
1	A	242	ARG
1	A	252	ARG
1	A	272	ARG
1	A	273	LEU
1	B	6	LEU
1	B	15	ARG
1	B	17	LEU
1	B	20	THR
1	B	25	LYS
1	B	31	VAL
1	B	57	ARG
1	B	59	LYS
1	B	60	ARG
1	B	61	SER
1	B	75	GLN
1	B	76	ILE
1	B	77	GLN
1	B	83	ASN
1	B	89	ARG
1	B	101	ARG
1	B	103	LYS
1	B	104	GLN
1	B	113	LEU
1	B	134	ILE
1	B	142	LEU
1	B	164	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	165	GLU
1	B	167	VAL
1	B	193	ASN
1	B	195	GLU
1	B	207	TYR
1	B	217	LEU
1	B	227	GLU
1	B	229	GLN
1	B	230	ILE
1	B	235	ARG
1	B	242	ARG
1	B	243	ILE
1	B	252	ARG
1	B	258	VAL
1	B	265	SER
1	C	1	MET
1	C	6	LEU
1	C	12	TYR
1	C	17	LEU
1	C	20	THR
1	C	31	VAL
1	C	57	ARG
1	C	59	LYS
1	C	62	LEU
1	C	70	TYR
1	C	74	HIS
1	C	76	ILE
1	C	81	LYS
1	C	101	ARG
1	C	103	LYS
1	C	104	GLN
1	C	105	MET
1	C	143	LYS
1	C	148	LEU
1	C	157	VAL
1	C	201	LEU
1	C	204	ILE
1	C	217	LEU
1	C	230	ILE
1	C	241	LYS
1	C	242	ARG
1	C	252	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3	LYS
1	D	6	LEU
1	D	35	LEU
1	D	57	ARG
1	D	59	LYS
1	D	60	ARG
1	D	68	THR
1	D	75	GLN
1	D	76	ILE
1	D	83	ASN
1	D	101	ARG
1	D	102	GLN
1	D	103	LYS
1	D	105	MET
1	D	113	LEU
1	D	128	LEU
1	D	130	ASP
1	D	136	HIS
1	D	142	LEU
1	D	148	LEU
1	D	150	GLN
1	D	157	VAL
1	D	164	LEU
1	D	173	ILE
1	D	195	GLU
1	D	201	LEU
1	D	204	ILE
1	D	217	LEU
1	D	227	GLU
1	D	230	ILE
1	D	241	LYS
1	D	242	ARG
1	D	252	ARG
1	D	270	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	80	ASN
1	A	83	ASN
1	A	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	GLN
1	A	110	HIS
1	A	136	HIS
1	A	225	ASN
1	A	229	GLN
1	B	77	GLN
1	B	83	ASN
1	B	102	GLN
1	B	193	ASN
1	B	194	GLN
1	B	229	GLN
1	C	77	GLN
1	C	80	ASN
1	C	102	GLN
1	C	153	GLN
1	C	200	ASN
1	C	225	ASN
1	C	226	ASN
1	C	229	GLN
1	C	247	GLN
1	D	58	ASN
1	D	75	GLN
1	D	77	GLN
1	D	83	ASN
1	D	90	ASN
1	D	102	GLN
1	D	136	HIS
1	D	150	GLN
1	D	247	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	273/281 (97%)	0.01	6 (2%)	62	59	34, 55, 83, 101	0
1	B	273/281 (97%)	0.11	14 (5%)	28	24	31, 54, 99, 113	0
1	C	273/281 (97%)	0.19	18 (6%)	18	14	34, 51, 99, 132	0
1	D	273/281 (97%)	0.19	14 (5%)	28	24	35, 55, 93, 107	0
All	All	1092/1124 (97%)	0.13	52 (4%)	30	27	31, 54, 94, 132	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	ASN	5.0
1	A	226	ASN	4.6
1	C	226	ASN	4.6
1	B	226	ASN	4.5
1	C	72	ILE	4.4
1	C	78	GLY	4.4
1	B	225	ASN	4.4
1	C	71	GLU	4.3
1	C	222	PRO	4.0
1	C	76	ILE	3.9
1	C	75	GLN	3.9
1	C	79	THR	3.9
1	B	223	GLY	3.8
1	B	224	LYS	3.7
1	D	74	HIS	3.7
1	D	80	ASN	3.6
1	D	105	MET	3.5
1	D	78	GLY	3.3
1	B	137	ASP	3.0
1	B	227	GLU	3.0
1	C	223	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	105	MET	2.9
1	D	79	THR	2.8
1	B	271	LYS	2.7
1	D	73	GLU	2.7
1	B	167	VAL	2.7
1	B	77	GLN	2.7
1	D	70	TYR	2.7
1	A	221	LYS	2.7
1	C	73	GLU	2.6
1	D	1	MET	2.5
1	C	74	HIS	2.5
1	C	81	LYS	2.5
1	C	273	LEU	2.5
1	D	194	GLN	2.4
1	D	268	TYR	2.4
1	A	1	MET	2.4
1	D	164	LEU	2.4
1	B	136	HIS	2.3
1	D	81	LYS	2.3
1	C	137	ASP	2.3
1	A	224	LYS	2.3
1	A	148	LEU	2.3
1	C	77	GLN	2.2
1	A	220	THR	2.2
1	B	78	GLY	2.2
1	D	167	VAL	2.2
1	B	165	GLU	2.1
1	B	248	PHE	2.1
1	C	220	THR	2.0
1	D	72	ILE	2.0
1	B	249	LYS	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.