Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:19 PM GMT

PDB ID	:	4HYY
Title	:	Filament of octameric rings of DMC1 recombinase from Homo sapiens
Authors	:	Du, L.; Luo, Y.
Deposited on	:	2012-11-14
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

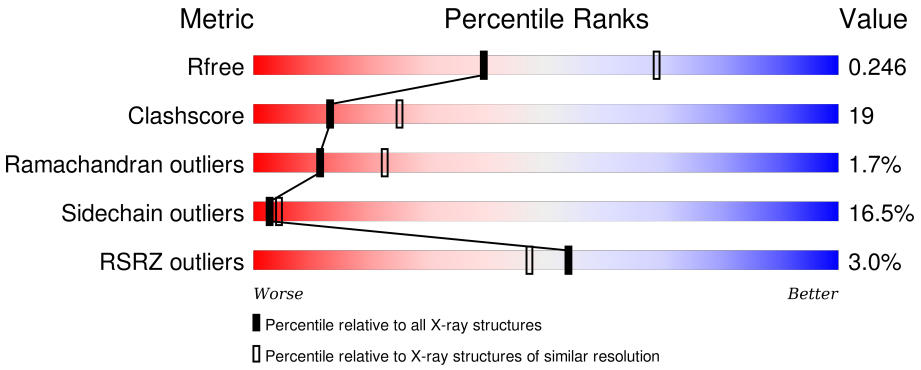
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	265	3% 60% 24% 6% 9%
1	B	265	3% 57% 26% 8% 9%
1	C	265	3% 56% 29% 6% 9%
1	D	265	3% 55% 26% 8% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7632 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 Meiotic recombination protein DMC1/LIM15 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			
1	B	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			
1	C	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			
1	D	241	Total	C	N	O	S	0	0	0
			1884	1193	327	356	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	LEU	-	EXPRESSION TAG	UNP Q14565
A	342	GLU	-	EXPRESSION TAG	UNP Q14565
A	343	HIS	-	EXPRESSION TAG	UNP Q14565
A	344	HIS	-	EXPRESSION TAG	UNP Q14565
A	345	HIS	-	EXPRESSION TAG	UNP Q14565
A	346	HIS	-	EXPRESSION TAG	UNP Q14565
A	347	HIS	-	EXPRESSION TAG	UNP Q14565
A	348	HIS	-	EXPRESSION TAG	UNP Q14565
B	341	LEU	-	EXPRESSION TAG	UNP Q14565
B	342	GLU	-	EXPRESSION TAG	UNP Q14565
B	343	HIS	-	EXPRESSION TAG	UNP Q14565
B	344	HIS	-	EXPRESSION TAG	UNP Q14565
B	345	HIS	-	EXPRESSION TAG	UNP Q14565
B	346	HIS	-	EXPRESSION TAG	UNP Q14565
B	347	HIS	-	EXPRESSION TAG	UNP Q14565
B	348	HIS	-	EXPRESSION TAG	UNP Q14565
C	341	LEU	-	EXPRESSION TAG	UNP Q14565
C	342	GLU	-	EXPRESSION TAG	UNP Q14565
C	343	HIS	-	EXPRESSION TAG	UNP Q14565
C	344	HIS	-	EXPRESSION TAG	UNP Q14565
C	345	HIS	-	EXPRESSION TAG	UNP Q14565

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	346	HIS	-	EXPRESSION TAG	UNP Q14565
C	347	HIS	-	EXPRESSION TAG	UNP Q14565
C	348	HIS	-	EXPRESSION TAG	UNP Q14565
D	341	LEU	-	EXPRESSION TAG	UNP Q14565
D	342	GLU	-	EXPRESSION TAG	UNP Q14565
D	343	HIS	-	EXPRESSION TAG	UNP Q14565
D	344	HIS	-	EXPRESSION TAG	UNP Q14565
D	345	HIS	-	EXPRESSION TAG	UNP Q14565
D	346	HIS	-	EXPRESSION TAG	UNP Q14565
D	347	HIS	-	EXPRESSION TAG	UNP Q14565
D	348	HIS	-	EXPRESSION TAG	UNP Q14565

- Molecule 2 is water.

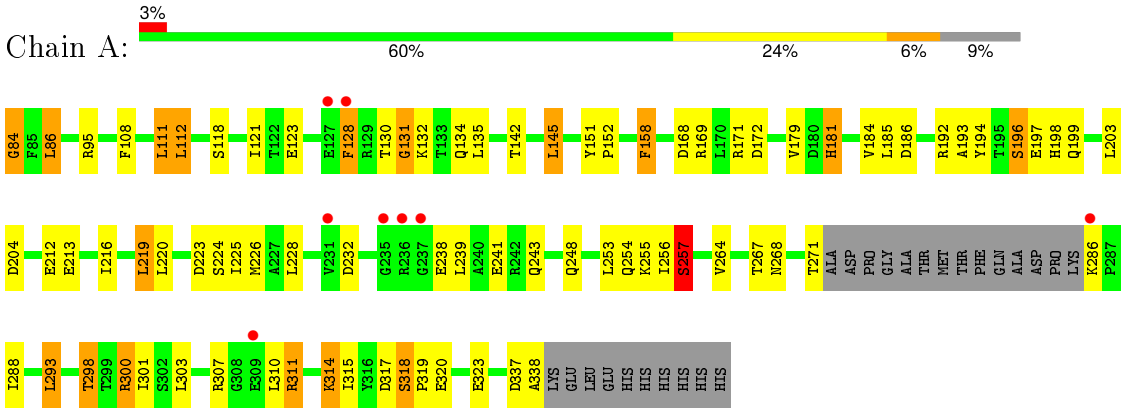
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	22	Total O 22 22	0	0
2	C	29	Total O 29 29	0	0
2	D	16	Total O 16 16	0	0

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.

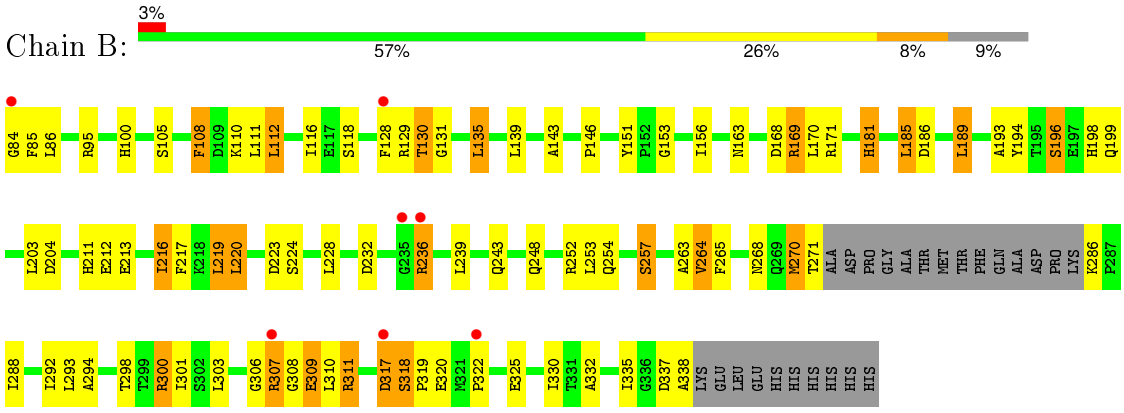
- Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

Chain A:



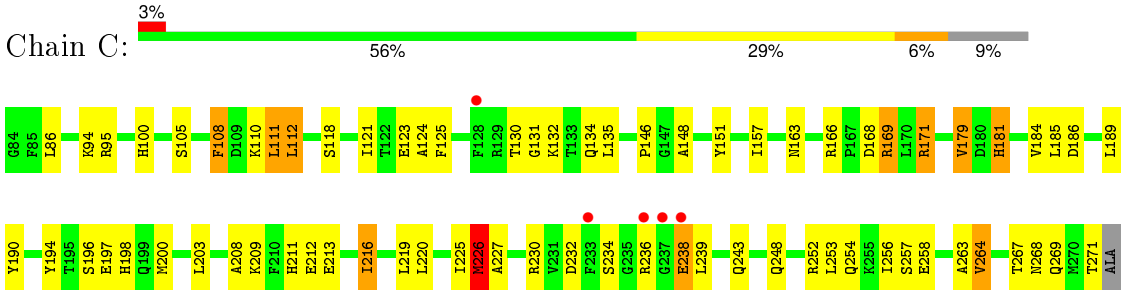
- Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

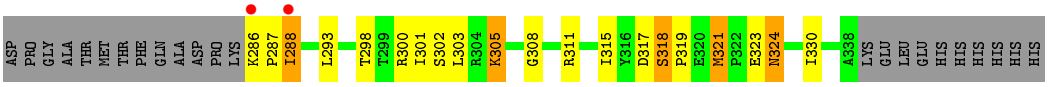
Chain B:



- Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

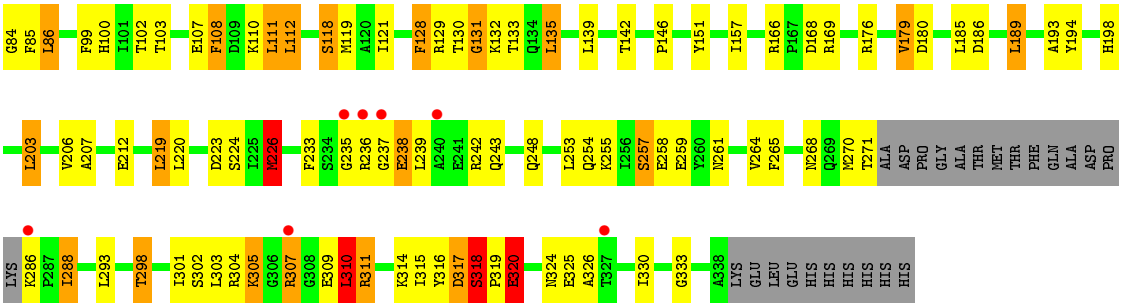
Chain C:





• Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	124.00Å 124.00Å 91.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.45 – 2.60 47.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.45-2.60) 96.3 (47.45-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.179 , 0.246 0.178 , 0.246	Depositor DCC
R_{free} test set	2157 reflections (5.52%)	DCC
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.9	EDS
Estimated twinning fraction	0.072 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 41190 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7632	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.82	1/1917 (0.1%)	1.01	7/2579 (0.3%)
1	B	0.77	1/1917 (0.1%)	0.92	2/2579 (0.1%)
1	C	0.74	0/1917	0.95	2/2579 (0.1%)
1	D	0.76	1/1917 (0.1%)	0.96	5/2579 (0.2%)
All	All	0.77	3/7668 (0.0%)	0.96	16/10316 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	84	GLY	N-CA	5.78	1.54	1.46
1	B	84	GLY	N-CA	5.75	1.54	1.46
1	A	84	GLY	N-CA	5.41	1.54	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	310	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	95	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	95	ARG	CG-CD-NE	-6.17	98.84	111.80
1	C	226	MET	CB-CA-C	-6.17	98.06	110.40
1	D	166	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	C	171	ARG	CB-CA-C	5.98	122.37	110.40
1	A	293	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	A	219	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	204	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	226	MET	CB-CG-SD	-5.27	96.59	112.40
1	A	257	SER	N-CA-CB	-5.21	102.68	110.50
1	D	226	MET	CB-CA-C	-5.19	100.02	110.40
1	D	235	GLY	N-CA-C	-5.14	100.24	113.10
1	D	166	ARG	CG-CD-NE	-5.14	101.01	111.80
1	B	95	ARG	CG-CD-NE	-5.06	101.18	111.80
1	B	257	SER	N-CA-CB	-5.01	102.98	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1884	0	1870	68	0
1	B	1884	0	1870	74	0
1	C	1884	0	1870	66	0
1	D	1884	0	1870	81	0
2	A	29	0	0	11	0
2	B	22	0	0	8	0
2	C	29	0	0	10	0
2	D	16	0	0	5	0
All	All	7632	0	7480	285	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 19.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:SER:HB3	1:B:319:PRO:HA	1.22	1.15
2:A:428:HOH:O	1:D:212:GLU:HG3	1.49	1.12
1:C:130:THR:HG21	1:C:303:LEU:HB3	1.19	1.12
1:C:318:SER:HB3	1:C:319:PRO:HA	1.21	1.11
1:A:318:SER:HB3	1:A:319:PRO:CA	1.80	1.11
1:C:212:GLU:HG2	2:C:429:HOH:O	1.49	1.10
1:B:311:ARG:HG2	1:B:311:ARG:HH11	0.99	1.08
1:A:318:SER:HB3	1:A:319:PRO:HA	1.11	1.06
1:D:318:SER:HB3	1:D:319:PRO:HA	1.31	1.04
1:B:318:SER:HB3	1:B:319:PRO:CA	1.89	1.02
1:D:130:THR:HG21	1:D:303:LEU:HB3	1.41	1.01
1:B:286:LYS:N	2:B:406:HOH:O	1.92	1.00
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.28	0.97
1:D:318:SER:HB3	1:D:319:PRO:CA	1.94	0.97
1:A:311:ARG:CG	1:A:311:ARG:HH11	1.77	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HG21	1:B:303:LEU:HB3	1.45	0.97
1:C:286:LYS:N	2:C:403:HOH:O	1.97	0.96
1:C:169:ARG:HG3	1:C:169:ARG:HH11	1.33	0.94
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.31	0.94
1:A:311:ARG:HH11	1:A:311:ARG:HG2	1.29	0.92
1:B:311:ARG:HG2	1:B:311:ARG:NH1	1.77	0.92
1:D:100:HIS:HD2	2:D:408:HOH:O	1.52	0.92
1:B:100:HIS:HD2	2:B:416:HOH:O	1.52	0.92
1:C:130:THR:HG21	1:C:303:LEU:CB	1.99	0.92
1:A:318:SER:CB	1:A:319:PRO:HA	1.99	0.91
1:B:130:THR:HG22	1:B:131:GLY:H	1.36	0.91
1:A:197:GLU:HG3	2:A:404:HOH:O	1.72	0.90
1:A:130:THR:HG21	1:A:303:LEU:HB3	1.54	0.89
1:C:130:THR:CG2	1:C:303:LEU:HB3	2.04	0.87
1:C:318:SER:HB3	1:C:319:PRO:CA	2.05	0.87
1:C:216:ILE:HD11	2:C:424:HOH:O	1.74	0.87
1:D:130:THR:HG22	1:D:131:GLY:N	1.88	0.85
1:A:130:THR:HA	1:A:311:ARG:HH12	1.41	0.85
1:D:239:LEU:O	1:D:243:GLN:HG2	1.76	0.85
1:A:254:GLN:O	1:A:257:SER:HB3	1.78	0.84
1:D:128:PHE:HZ	1:D:133:THR:HG1	0.85	0.84
1:B:216:ILE:H	1:B:216:ILE:HD12	1.41	0.83
1:D:128:PHE:HZ	1:D:133:THR:OG1	1.61	0.83
1:C:318:SER:CB	1:C:319:PRO:HA	2.06	0.83
1:A:142:THR:HA	1:A:145:LEU:HD22	1.62	0.81
1:A:130:THR:HG21	1:A:303:LEU:CB	2.11	0.81
1:C:194:TYR:H	1:C:198:HIS:HD2	1.28	0.80
1:A:239:LEU:O	1:A:243:GLN:HG2	1.83	0.79
1:C:112:LEU:HD11	1:C:301:ILE:HD11	1.66	0.78
1:C:171:ARG:HE	1:C:181:HIS:HB2	1.48	0.77
1:A:194:TYR:H	1:A:198:HIS:HD2	1.30	0.77
1:D:130:THR:HA	1:D:311:ARG:HE	1.49	0.77
1:B:311:ARG:HH11	1:B:311:ARG:CG	1.88	0.77
1:D:130:THR:HG22	1:D:131:GLY:H	1.46	0.77
1:D:121:ILE:H	1:D:298:THR:HG23	1.49	0.77
1:B:171:ARG:HG2	1:B:181:HIS:HB3	1.67	0.76
1:B:239:LEU:O	1:B:243:GLN:HG2	1.85	0.76
1:B:298:THR:HG23	2:B:405:HOH:O	1.85	0.75
1:A:216:ILE:HD11	2:A:403:HOH:O	1.85	0.75
1:D:233:PHE:HB2	1:D:242:ARG:HB2	1.69	0.75
1:D:314:LYS:HD3	1:D:325:GLU:HG2	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LEU:O	1:C:243:GLN:HG2	1.87	0.75
1:C:319:PRO:HD2	1:C:324:ASN:ND2	2.02	0.74
1:D:311:ARG:CG	1:D:311:ARG:HH11	2.01	0.73
1:B:130:THR:HG21	1:B:303:LEU:CB	2.18	0.73
1:B:131:GLY:N	1:B:311:ARG:HH12	1.87	0.72
1:D:307:ARG:O	1:D:310:LEU:HD13	1.90	0.72
1:B:194:TYR:H	1:B:198:HIS:HD2	1.38	0.71
1:A:130:THR:CG2	1:A:303:LEU:HB3	2.21	0.71
1:B:216:ILE:HD13	1:B:217:PHE:H	1.54	0.71
1:B:169:ARG:CG	1:B:169:ARG:HH11	2.01	0.71
1:C:238:GLU:HA	1:C:238:GLU:OE1	1.89	0.71
1:C:213:GLU:HB3	1:C:216:ILE:HD12	1.72	0.70
1:A:112:LEU:HD11	1:A:301:ILE:HD11	1.73	0.70
1:B:110:LYS:HG3	1:B:111:LEU:N	2.06	0.69
1:B:254:GLN:O	1:B:257:SER:HB3	1.93	0.69
1:C:163:ASN:HD22	1:D:298:THR:HG21	1.58	0.68
1:A:298:THR:HG21	1:B:163:ASN:HD22	1.59	0.68
1:C:254:GLN:O	1:C:257:SER:HB3	1.93	0.68
1:D:194:TYR:H	1:D:198:HIS:HD2	1.39	0.68
1:A:130:THR:HG22	1:A:131:GLY:N	2.09	0.67
1:B:309:GLU:HB2	1:B:330:ILE:HD11	1.77	0.67
1:D:130:THR:CG2	1:D:131:GLY:H	2.09	0.66
1:A:311:ARG:NH1	1:A:311:ARG:HG2	2.07	0.66
1:B:130:THR:CG2	1:B:303:LEU:HB3	2.24	0.66
1:C:111:LEU:HD22	1:C:315:ILE:CD1	2.26	0.65
1:B:338:ALA:HB1	2:B:420:HOH:O	1.96	0.65
1:D:100:HIS:CD2	2:D:408:HOH:O	2.36	0.65
1:D:111:LEU:HD22	1:D:315:ILE:CD1	2.27	0.65
1:C:319:PRO:HD2	1:C:324:ASN:HD21	1.61	0.64
1:B:196:SER:HB2	1:B:232:ASP:OD2	1.97	0.64
1:B:306:GLY:O	1:B:308:GLY:N	2.31	0.64
1:A:130:THR:HG22	1:A:131:GLY:H	1.62	0.63
1:A:84:GLY:O	2:A:419:HOH:O	2.16	0.62
1:C:100:HIS:HD2	2:C:406:HOH:O	1.80	0.62
1:C:252:ARG:O	1:C:256:ILE:HG13	1.98	0.62
1:D:307:ARG:HH11	1:D:307:ARG:HB2	1.64	0.62
1:B:131:GLY:H	1:B:311:ARG:HH12	1.45	0.62
1:A:213:GLU:N	2:A:403:HOH:O	2.31	0.62
1:A:123:GLU:OE1	1:A:300:ARG:HD2	2.00	0.62
1:A:130:THR:HA	1:A:311:ARG:NH1	2.12	0.61
1:B:216:ILE:HD13	1:B:217:PHE:N	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:LEU:HD22	1:D:315:ILE:HD11	1.83	0.61
1:B:130:THR:HG22	1:B:131:GLY:N	2.13	0.60
1:C:125:PHE:HB3	1:C:268:ASN:HB3	1.82	0.60
1:D:112:LEU:HD11	1:D:301:ILE:HD11	1.84	0.60
1:A:172:ASP:HB3	2:A:413:HOH:O	2.01	0.59
1:A:310:LEU:C	1:A:311:ARG:HD2	2.22	0.59
1:C:230:ARG:O	1:C:234:SER:HB3	2.02	0.59
1:D:233:PHE:CB	1:D:242:ARG:HB2	2.32	0.59
1:C:194:TYR:H	1:C:198:HIS:CD2	2.17	0.59
1:C:123:GLU:OE1	1:C:300:ARG:HD2	2.02	0.59
1:A:225:ILE:HG22	1:A:267:THR:O	2.03	0.59
1:C:186:ASP:HB3	2:C:419:HOH:O	2.02	0.58
1:A:298:THR:CG2	2:A:402:HOH:O	2.51	0.58
1:A:171:ARG:HG2	1:A:181:HIS:HB3	1.84	0.58
1:B:216:ILE:HD12	1:B:216:ILE:N	2.16	0.57
1:D:268:ASN:ND2	2:D:405:HOH:O	2.34	0.57
1:D:311:ARG:CG	1:D:311:ARG:NH1	2.65	0.57
1:C:323:GLU:HA	2:C:423:HOH:O	2.03	0.57
1:D:319:PRO:O	1:D:320:GLU:HB2	2.04	0.57
1:D:318:SER:HB3	1:D:319:PRO:C	2.24	0.57
1:C:110:LYS:HD3	2:C:418:HOH:O	2.05	0.57
1:D:318:SER:CB	1:D:319:PRO:HA	2.20	0.56
1:D:238:GLU:O	1:D:238:GLU:HG2	2.05	0.56
1:B:105:SER:HB3	1:B:108:PHE:HB2	1.86	0.56
1:D:111:LEU:CD2	1:D:315:ILE:CD1	2.84	0.56
1:C:130:THR:HG22	1:C:131:GLY:N	2.22	0.55
1:B:216:ILE:CD1	1:B:217:PHE:H	2.19	0.55
1:B:204:ASP:OD1	1:B:252:ARG:NH2	2.35	0.55
1:A:194:TYR:H	1:A:198:HIS:CD2	2.20	0.54
1:C:111:LEU:HD22	1:C:315:ILE:HD13	1.89	0.54
1:A:199:GLN:HE21	1:A:228:LEU:HD12	1.71	0.54
1:C:148:ALA:HA	2:C:407:HOH:O	2.08	0.53
1:B:171:ARG:HG2	1:B:181:HIS:CB	2.36	0.53
1:B:292:ILE:HD12	2:B:421:HOH:O	2.08	0.53
1:C:169:ARG:CG	1:C:169:ARG:HH11	2.13	0.53
1:C:163:ASN:O	1:C:166:ARG:NH2	2.42	0.53
1:D:316:TYR:O	1:D:317:ASP:HB2	2.08	0.53
1:C:286:LYS:HG2	1:C:287:PRO:HD2	1.92	0.52
1:C:226:MET:HE2	1:C:288:ILE:HD13	1.91	0.52
1:C:134:GLN:HE22	1:C:169:ARG:NH1	2.07	0.52
1:D:146:PRO:HA	1:D:151:TYR:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LYS:HA	1:D:311:ARG:HG2	1.92	0.52
1:C:130:THR:HG22	1:C:131:GLY:H	1.75	0.51
1:A:123:GLU:OE1	1:A:300:ARG:CD	2.58	0.51
1:B:199:GLN:HE21	1:B:228:LEU:HD12	1.74	0.51
1:B:307:ARG:HB3	1:B:310:LEU:HD13	1.92	0.51
1:D:119:MET:HG2	1:D:258:GLU:HA	1.92	0.51
1:C:121:ILE:HG23	1:C:264:VAL:HG22	1.91	0.51
1:D:128:PHE:HZ	1:D:133:THR:CB	2.23	0.51
1:B:254:GLN:NE2	2:B:411:HOH:O	2.43	0.51
1:C:146:PRO:HA	1:C:151:TYR:O	2.11	0.51
1:B:216:ILE:CD1	1:B:216:ILE:H	2.17	0.51
1:D:194:TYR:H	1:D:198:HIS:CD2	2.25	0.51
1:D:135:LEU:HD13	1:D:265:PHE:CZ	2.46	0.50
1:A:311:ARG:CG	1:A:311:ARG:NH1	2.48	0.50
1:A:181:HIS:N	1:A:181:HIS:ND1	2.58	0.50
1:D:102:THR:HG23	1:D:142:THR:HB	1.93	0.50
1:D:236:ARG:HB2	1:D:239:LEU:HG	1.94	0.50
1:B:270:MET:HE3	2:B:422:HOH:O	2.11	0.49
1:D:318:SER:CB	1:D:319:PRO:CA	2.78	0.49
1:B:146:PRO:HA	1:B:151:TYR:O	2.12	0.49
1:B:271:THR:HG23	1:B:288:ILE:HG22	1.94	0.49
1:D:130:THR:HG23	1:D:311:ARG:HD3	1.94	0.48
1:A:311:ARG:HH11	1:A:311:ARG:HG3	1.69	0.48
1:A:86:LEU:HD23	1:A:86:LEU:H	1.77	0.48
1:C:171:ARG:NE	1:C:181:HIS:HB2	2.23	0.48
1:A:318:SER:HB3	1:A:319:PRO:C	2.33	0.48
1:A:130:THR:HG21	1:A:303:LEU:HB2	1.95	0.48
1:C:169:ARG:HG3	1:C:169:ARG:NH1	2.11	0.48
1:C:134:GLN:HE22	1:C:169:ARG:HH12	1.59	0.48
1:A:298:THR:HG21	1:B:163:ASN:ND2	2.25	0.48
1:D:307:ARG:NH1	1:D:307:ARG:HB2	2.28	0.47
1:C:226:MET:O	1:C:227:ALA:C	2.50	0.47
1:A:223:ASP:HA	1:A:224:SER:HA	1.74	0.47
1:B:211:HIS:CD2	2:B:407:HOH:O	2.68	0.47
1:B:151:TYR:CE2	1:B:153:GLY:HA2	2.50	0.47
1:A:196:SER:HB2	1:A:232:ASP:OD2	2.15	0.47
1:C:318:SER:CB	1:C:319:PRO:CA	2.78	0.47
1:B:311:ARG:NH1	1:B:311:ARG:CG	2.57	0.47
1:D:130:THR:CG2	1:D:131:GLY:N	2.59	0.46
1:B:112:LEU:HD11	1:B:301:ILE:HD11	1.97	0.46
1:A:314:LYS:NZ	1:A:320:GLU:OE2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HB3	1:B:219:LEU:HD11	1.98	0.46
1:D:226:MET:HB2	2:D:405:HOH:O	2.14	0.46
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.68	0.46
1:D:176:ARG:HD2	1:D:333:GLY:O	2.15	0.46
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.79	0.46
1:A:128:PHE:CD1	1:A:128:PHE:N	2.82	0.46
1:B:169:ARG:NH2	1:B:332:ALA:O	2.47	0.46
1:B:143:ALA:HB3	1:B:156:ILE:HD11	1.97	0.46
1:B:213:GLU:O	1:B:216:ILE:HD11	2.16	0.46
1:A:84:GLY:CA	2:A:419:HOH:O	2.63	0.46
1:C:118:SER:HA	1:C:263:ALA:HA	1.97	0.46
1:A:134:GLN:OE1	1:A:169:ARG:NH1	2.49	0.46
1:D:193:ALA:HA	1:D:198:HIS:CD2	2.51	0.46
1:B:337:ASP:O	1:B:338:ALA:C	2.55	0.45
1:C:226:MET:CE	1:C:288:ILE:HD13	2.47	0.45
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.83	0.45
1:C:169:ARG:HD2	1:C:169:ARG:HA	1.82	0.45
1:D:268:ASN:HD21	1:D:288:ILE:HD12	1.80	0.45
1:D:86:LEU:HD23	1:D:86:LEU:H	1.81	0.45
1:B:116:ILE:HG22	1:B:263:ALA:HB1	1.99	0.45
1:D:107:GLU:HB3	1:D:326:ALA:HB1	1.98	0.45
1:B:86:LEU:N	1:B:86:LEU:HD23	2.32	0.45
1:B:223:ASP:HA	1:B:224:SER:HA	1.67	0.45
1:D:103:THR:OG1	1:D:108:PHE:HB3	2.17	0.45
1:B:189:LEU:HD23	1:B:217:PHE:CZ	2.51	0.45
1:B:294:ALA:HB2	1:B:300:ARG:HH21	1.82	0.45
1:B:85:PHE:N	1:B:85:PHE:CD1	2.85	0.45
1:C:196:SER:HB2	1:C:232:ASP:OD2	2.17	0.44
1:C:94:LYS:NZ	1:C:258:GLU:O	2.50	0.44
1:C:321:MET:HB3	1:C:323:GLU:HG2	1.99	0.44
1:D:131:GLY:O	1:D:135:LEU:HB2	2.18	0.44
1:A:310:LEU:O	1:A:311:ARG:HD2	2.17	0.44
1:A:111:LEU:HD13	1:A:315:ILE:HD12	1.99	0.44
2:A:428:HOH:O	1:D:212:GLU:CG	2.30	0.44
1:D:318:SER:OG	1:D:320:GLU:N	2.51	0.44
1:D:319:PRO:HD2	1:D:324:ASN:ND2	2.33	0.44
1:A:193:ALA:HA	1:A:198:HIS:CD2	2.53	0.44
1:D:226:MET:HE3	1:D:226:MET:HB3	1.70	0.44
1:C:197:GLU:HB2	2:C:410:HOH:O	2.17	0.44
1:D:189:LEU:HD12	1:D:189:LEU:HA	1.87	0.44
1:A:286:LYS:N	2:A:423:HOH:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:HD21	1:A:288:ILE:HG13	1.82	0.44
1:A:268:ASN:HD21	1:A:288:ILE:CG1	2.30	0.43
1:C:105:SER:HB3	1:C:108:PHE:HB2	2.00	0.43
1:A:179:VAL:CG1	1:A:184:VAL:HG23	2.47	0.43
1:D:121:ILE:N	1:D:298:THR:HG23	2.27	0.43
1:D:132:LYS:HE3	1:D:132:LYS:HB2	1.83	0.43
1:B:253:LEU:HA	1:B:253:LEU:HD23	1.72	0.43
1:B:118:SER:HA	1:B:263:ALA:HA	2.00	0.43
1:D:179:VAL:HG12	1:D:180:ASP:H	1.84	0.43
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.80	0.43
1:B:317:ASP:O	1:B:318:SER:O	2.37	0.43
1:C:190:TYR:O	1:D:85:PHE:HA	2.19	0.43
1:C:225:ILE:HG23	1:C:226:MET:HG3	2.00	0.42
1:A:314:LYS:HE2	1:A:318:SER:HA	2.01	0.42
1:A:130:THR:CG2	1:A:131:GLY:N	2.79	0.42
1:C:330:ILE:O	1:C:330:ILE:HD12	2.19	0.42
1:B:220:LEU:HB3	1:B:264:VAL:HB	2.00	0.42
1:D:118:SER:OG	1:D:261:ASN:OD1	2.37	0.42
1:A:212:GLU:HG3	2:D:411:HOH:O	2.18	0.42
1:D:238:GLU:O	1:D:238:GLU:CG	2.67	0.42
1:C:253:LEU:HD23	1:C:253:LEU:HA	1.65	0.42
1:A:192:ARG:HD2	1:A:192:ARG:HH11	1.72	0.42
1:A:151:TYR:HA	1:A:152:PRO:HD3	1.93	0.42
1:D:226:MET:HE2	1:D:288:ILE:HD13	2.01	0.42
1:A:179:VAL:CG1	1:A:184:VAL:CG2	2.98	0.42
1:C:305:LYS:HB3	1:C:305:LYS:HE2	1.50	0.42
1:B:170:LEU:HD12	1:B:185:LEU:HD12	2.01	0.42
1:B:268:ASN:HD21	1:B:288:ILE:CG1	2.33	0.42
1:D:303:LEU:HA	1:D:303:LEU:HD23	1.81	0.42
1:B:236:ARG:HA	1:B:239:LEU:HD23	2.02	0.42
1:D:111:LEU:CD2	1:D:315:ILE:HD13	2.49	0.42
1:D:223:ASP:HA	1:D:224:SER:HA	1.77	0.42
1:B:330:ILE:H	1:B:330:ILE:HG13	1.76	0.41
1:D:130:THR:O	1:D:132:LYS:N	2.54	0.41
1:B:307:ARG:HA	1:B:307:ARG:HH11	1.84	0.41
1:D:255:LYS:O	1:D:259:GLU:HB2	2.20	0.41
1:D:139:LEU:HB3	1:D:219:LEU:HD11	2.03	0.41
1:A:319:PRO:HB3	2:A:415:HOH:O	2.19	0.41
1:C:179:VAL:CG1	1:C:184:VAL:HG23	2.50	0.41
1:A:194:TYR:N	1:A:198:HIS:HD2	2.10	0.41
1:C:268:ASN:ND2	1:C:269:GLN:H	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:C	1:A:158:PHE:CD2	2.94	0.41
1:B:105:SER:HB3	1:B:108:PHE:CB	2.51	0.41
1:D:99:PHE:CE1	1:D:118:SER:HB2	2.55	0.41
1:C:208:ALA:O	1:C:209:LYS:C	2.57	0.41
1:A:130:THR:CG2	1:A:131:GLY:H	2.31	0.41
1:B:135:LEU:HD13	1:B:265:PHE:CZ	2.56	0.41
1:A:121:ILE:HD11	1:A:253:LEU:HB3	2.02	0.41
1:D:236:ARG:HD2	1:D:239:LEU:HD11	2.03	0.41
1:A:337:ASP:O	1:A:338:ALA:C	2.58	0.41
1:B:322:PRO:O	1:B:325:GLU:N	2.46	0.41
1:A:131:GLY:O	1:A:132:LYS:C	2.59	0.40
1:B:193:ALA:HA	1:B:198:HIS:CD2	2.56	0.40
1:D:319:PRO:O	1:D:320:GLU:CB	2.69	0.40
1:C:132:LYS:HD2	1:C:267:THR:HB	2.03	0.40
1:C:130:THR:HG23	1:C:311:ARG:HD2	2.04	0.40
1:C:124:ALA:O	1:C:267:THR:HA	2.21	0.40
1:D:206:VAL:O	1:D:207:ALA:C	2.57	0.40
1:C:226:MET:HB2	2:C:401:HOH:O	2.22	0.40
1:D:169:ARG:HG3	1:D:169:ARG:HH11	1.85	0.40
1:B:169:ARG:HA	1:B:169:ARG:HD2	1.75	0.40
1:D:111:LEU:HD21	1:D:315:ILE:HD13	2.04	0.40
1:A:86:LEU:N	1:A:86:LEU:HD23	2.37	0.40
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.71	0.40
1:D:254:GLN:O	1:D:257:SER:HB3	2.21	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	237/265 (89%)	221 (93%)	11 (5%)	5 (2%)	9 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	237/265 (89%)	219 (92%)	14 (6%)	4 (2%)	11 22
1	C	237/265 (89%)	230 (97%)	5 (2%)	2 (1%)	24 46
1	D	237/265 (89%)	220 (93%)	12 (5%)	5 (2%)	9 16
All	All	948/1060 (89%)	890 (94%)	42 (4%)	16 (2%)	11 22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	SER
1	B	128	PHE
1	B	307	ARG
1	B	318	SER
1	D	317	ASP
1	D	318	SER
1	A	257	SER
1	B	320	GLU
1	C	318	SER
1	D	131	GLY
1	D	320	GLU
1	A	131	GLY
1	D	237	GLY
1	A	238	GLU
1	C	308	GLY
1	A	256	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	196/216 (91%)	166 (85%)	30 (15%)	3 5
1	B	196/216 (91%)	169 (86%)	27 (14%)	4 7
1	C	196/216 (91%)	163 (83%)	33 (17%)	2 4
1	D	196/216 (91%)	157 (80%)	39 (20%)	1 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	784/864 (91%)	655 (84%)	129 (16%)	3 4

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	108	PHE
1	A	111	LEU
1	A	112	LEU
1	A	118	SER
1	A	128	PHE
1	A	135	LEU
1	A	145	LEU
1	A	158	PHE
1	A	168	ASP
1	A	181	HIS
1	A	185	LEU
1	A	186	ASP
1	A	196	SER
1	A	203	LEU
1	A	219	LEU
1	A	220	LEU
1	A	241	GLU
1	A	248	GLN
1	A	255	LYS
1	A	264	VAL
1	A	271	THR
1	A	293	LEU
1	A	298	THR
1	A	300	ARG
1	A	307	ARG
1	A	311	ARG
1	A	314	LYS
1	A	317	ASP
1	A	323	GLU
1	B	108	PHE
1	B	112	LEU
1	B	129	ARG
1	B	130	THR
1	B	135	LEU
1	B	168	ASP
1	B	169	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	181	HIS
1	B	185	LEU
1	B	186	ASP
1	B	189	LEU
1	B	196	SER
1	B	203	LEU
1	B	212	GLU
1	B	216	ILE
1	B	219	LEU
1	B	220	LEU
1	B	236	ARG
1	B	248	GLN
1	B	264	VAL
1	B	270	MET
1	B	293	LEU
1	B	300	ARG
1	B	309	GLU
1	B	311	ARG
1	B	317	ASP
1	B	335	ILE
1	C	86	LEU
1	C	95	ARG
1	C	108	PHE
1	C	111	LEU
1	C	112	LEU
1	C	135	LEU
1	C	157	ILE
1	C	168	ASP
1	C	169	ARG
1	C	179	VAL
1	C	181	HIS
1	C	185	LEU
1	C	189	LEU
1	C	200	MET
1	C	203	LEU
1	C	211	HIS
1	C	216	ILE
1	C	219	LEU
1	C	220	LEU
1	C	226	MET
1	C	236	ARG
1	C	238	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	248	GLN
1	C	264	VAL
1	C	271	THR
1	C	288	ILE
1	C	293	LEU
1	C	298	THR
1	C	302	SER
1	C	305	LYS
1	C	317	ASP
1	C	321	MET
1	C	324	ASN
1	D	86	LEU
1	D	108	PHE
1	D	110	LYS
1	D	111	LEU
1	D	112	LEU
1	D	118	SER
1	D	128	PHE
1	D	129	ARG
1	D	135	LEU
1	D	157	ILE
1	D	168	ASP
1	D	179	VAL
1	D	185	LEU
1	D	186	ASP
1	D	189	LEU
1	D	203	LEU
1	D	219	LEU
1	D	220	LEU
1	D	226	MET
1	D	238	GLU
1	D	248	GLN
1	D	257	SER
1	D	264	VAL
1	D	270	MET
1	D	271	THR
1	D	286	LYS
1	D	288	ILE
1	D	293	LEU
1	D	298	THR
1	D	302	SER
1	D	304	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	305	LYS
1	D	307	ARG
1	D	309	GLU
1	D	310	LEU
1	D	311	ARG
1	D	318	SER
1	D	320	GLU
1	D	330	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	199	GLN
1	A	254	GLN
1	A	268	ASN
1	A	324	ASN
1	B	163	ASN
1	B	198	HIS
1	B	199	GLN
1	B	268	ASN
1	B	269	GLN
1	C	134	GLN
1	C	163	ASN
1	C	198	HIS
1	C	199	GLN
1	C	268	ASN
1	C	324	ASN
1	D	198	HIS
1	D	199	GLN
1	D	254	GLN
1	D	268	ASN
1	D	324	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	241/265 (90%)	-0.11	8 (3%)	50	43	32, 54, 111, 139	0
1	B	241/265 (90%)	0.06	7 (2%)	55	48	35, 64, 120, 158	0
1	C	241/265 (90%)	-0.09	7 (2%)	55	48	32, 61, 113, 155	0
1	D	241/265 (90%)	0.09	7 (2%)	55	48	38, 64, 123, 162	0
All	All	964/1060 (90%)	-0.01	29 (3%)	54	47	32, 61, 119, 162	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	ARG	4.8
1	A	128	PHE	4.6
1	B	236	ARG	4.5
1	C	236	ARG	4.1
1	A	127	GLU	4.0
1	D	236	ARG	3.8
1	B	128	PHE	3.8
1	D	307	ARG	3.6
1	C	237	GLY	3.3
1	B	317	ASP	3.0
1	C	128	PHE	3.0
1	A	309	GLU	2.9
1	A	286	LYS	2.8
1	C	286	LYS	2.7
1	B	322	PRO	2.6
1	D	237	GLY	2.6
1	C	288	ILE	2.6
1	D	235	GLY	2.5
1	D	327	THR	2.5
1	A	235	GLY	2.5
1	B	307	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	2.4
1	B	235	GLY	2.3
1	C	238	GLU	2.3
1	D	240	ALA	2.2
1	A	231	VAL	2.2
1	D	286	LYS	2.1
1	B	84	GLY	2.1
1	C	233	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.