Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 07:08 PM EDT

PDB ID	:	4OSK
Title	:	Crystal structure of TAL effector reveals the recognition between asparagine and guanine
Authors	:	Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.
Deposited on	:	2014-02-13
Resolution	:	2.40 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 ⓘ 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 ⓘ) were used in the production of this report:

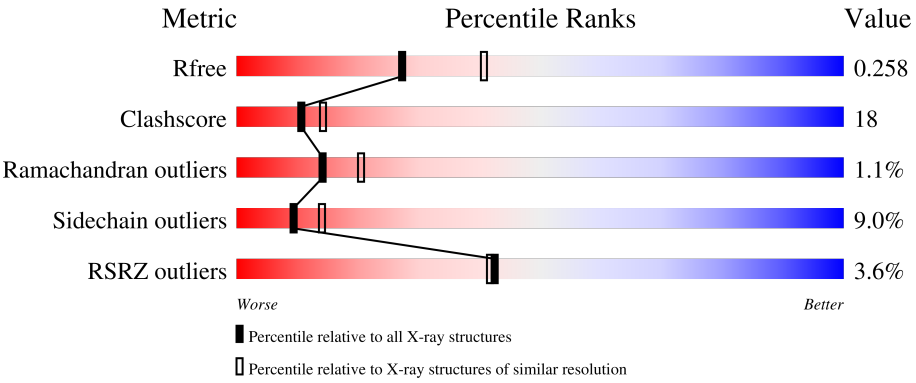
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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.



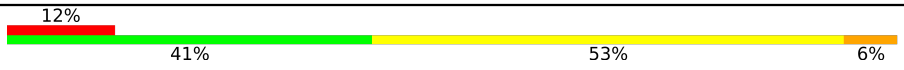
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	499	4% 65% 30%
1	B	499	3% 63% 30% 5%
2	G	17	65% 18% 12% 6%
2	I	17	6% 53% 41% 6%
3	H	17	12% 65% 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	17	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8734 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 Hax3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	5	1	0
			3551	2215	659	665	12			
1	B	491	Total	C	N	O	S	5	0	0
			3561	2224	659	665	13			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	-	expression tag	UNP Q3ZD72
A	300	HIS	ASN	engineered mutation	UNP Q3ZD72
A	301	ASP	ILE	engineered mutation	UNP Q3ZD72
A	369	SER	ILE	engineered mutation	UNP Q3ZD72
A	402	ASN	HIS	engineered mutation	UNP Q3ZD72
A	403	SER	ASP	engineered mutation	UNP Q3ZD72
A	470	ASN	HIS	engineered mutation	UNP Q3ZD72
A	471	GLY	ASP	engineered mutation	UNP Q3ZD72
A	538	HIS	ASN	engineered mutation	UNP Q3ZD72
A	539	ASP	SER	engineered mutation	UNP Q3ZD72
A	573	GLY	SER	engineered mutation	UNP Q3ZD72
A	606	ASN	HIS	engineered mutation	UNP Q3ZD72
A	607	SER	ASP	engineered mutation	UNP Q3ZD72
A	641	ASN	ILE	engineered mutation	UNP Q3ZD72
A	675	SER	GLY	engineered mutation	UNP Q3ZD72
A	721	LEU	-	expression tag	UNP Q3ZD72
A	722	GLU	-	expression tag	UNP Q3ZD72
A	723	HIS	-	expression tag	UNP Q3ZD72
A	724	HIS	-	expression tag	UNP Q3ZD72
A	725	HIS	-	expression tag	UNP Q3ZD72
A	726	HIS	-	expression tag	UNP Q3ZD72
A	727	HIS	-	expression tag	UNP Q3ZD72
A	728	HIS	-	expression tag	UNP Q3ZD72
B	230	MET	-	expression tag	UNP Q3ZD72
B	300	HIS	ASN	engineered mutation	UNP Q3ZD72

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	301	ASP	ILE	engineered mutation	UNP Q3ZD72
B	369	SER	ILE	engineered mutation	UNP Q3ZD72
B	402	ASN	HIS	engineered mutation	UNP Q3ZD72
B	403	SER	ASP	engineered mutation	UNP Q3ZD72
B	470	ASN	HIS	engineered mutation	UNP Q3ZD72
B	471	GLY	ASP	engineered mutation	UNP Q3ZD72
B	538	HIS	ASN	engineered mutation	UNP Q3ZD72
B	539	ASP	SER	engineered mutation	UNP Q3ZD72
B	573	GLY	SER	engineered mutation	UNP Q3ZD72
B	606	ASN	HIS	engineered mutation	UNP Q3ZD72
B	607	SER	ASP	engineered mutation	UNP Q3ZD72
B	641	ASN	ILE	engineered mutation	UNP Q3ZD72
B	675	SER	GLY	engineered mutation	UNP Q3ZD72
B	721	LEU	-	expression tag	UNP Q3ZD72
B	722	GLU	-	expression tag	UNP Q3ZD72
B	723	HIS	-	expression tag	UNP Q3ZD72
B	724	HIS	-	expression tag	UNP Q3ZD72
B	725	HIS	-	expression tag	UNP Q3ZD72
B	726	HIS	-	expression tag	UNP Q3ZD72
B	727	HIS	-	expression tag	UNP Q3ZD72
B	728	HIS	-	expression tag	UNP Q3ZD72

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*AP*AP*CP*TP*AP*CP*TP*AP*GP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			341	165	60	100	16			
2	G	16	Total	C	N	O	P	0	0	0
			321	155	58	93	15			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*TP*CP*TP*AP*GP*TP*AP*GP*TP*TP*GP*GP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	17	Total	C	N	O	P	0	0	0
			350	168	66	100	16			
3	H	17	Total	C	N	O	P	0	0	0
			350	168	66	100	16			

- Molecule 4 is water.

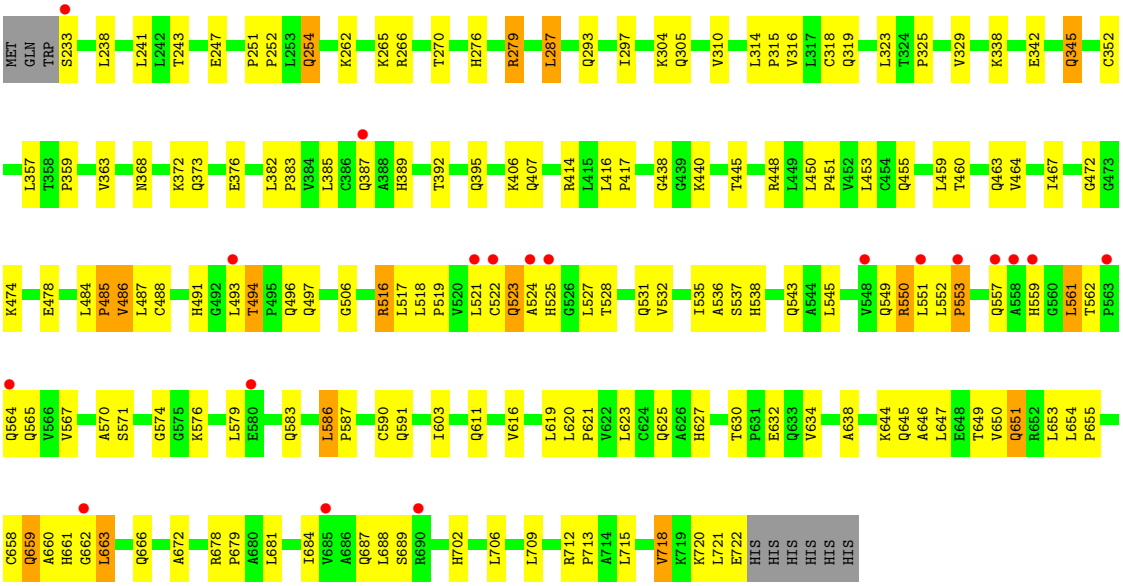
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	99	Total O 99 99	0	0
4	I	27	Total O 27 27	0	0
4	J	7	Total O 7 7	0	0
4	B	90	Total O 90 90	0	0
4	G	24	Total O 24 24	0	0
4	H	13	Total O 13 13	0	0

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.

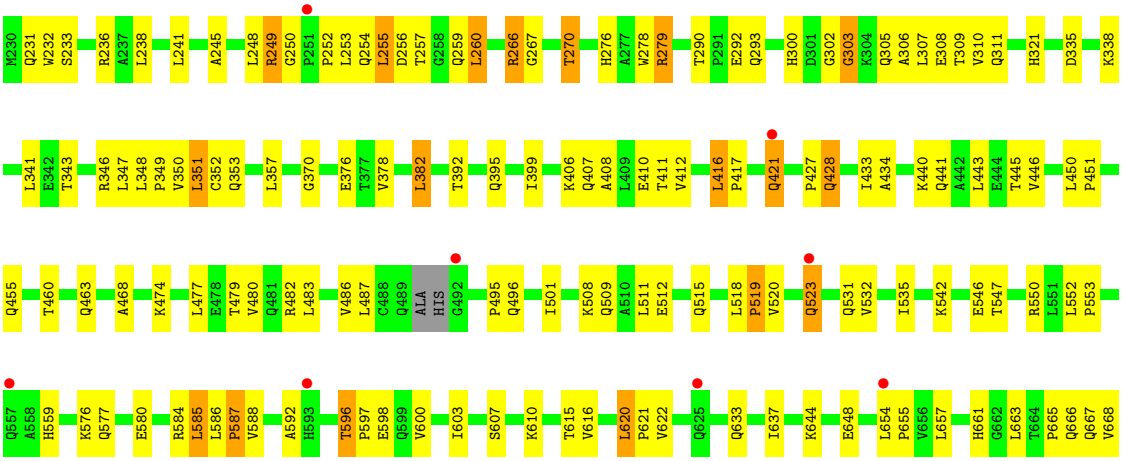
• Molecule 1: Hax3

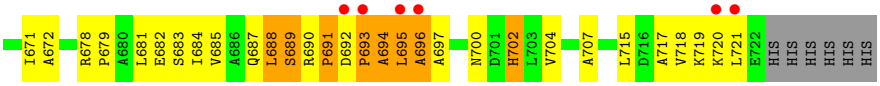
Chain A:



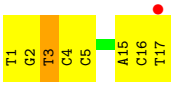
• Molecule 1: Hax3

Chain B:

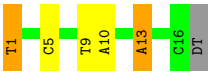




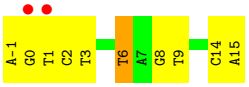
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*AP*AP*CP*TP*AP*CP*TP*AP*GP*AP*CP *T)-3')



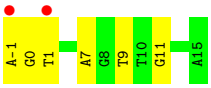
• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*AP*AP*CP*TP*AP*CP*TP*AP*GP*AP*CP *T)-3')



• Molecule 3: DNA (5'-D(*AP*GP*TP*CP*TP*AP*GP*TP*AP*GP*TP*TP*GP*GP*AP*CP *A)-3')



• Molecule 3: DNA (5'-D(*AP*GP*TP*CP*TP*AP*GP*TP*AP*GP*TP*TP*GP*GP*AP*CP *A)-3')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.63Å 88.13Å 90.48Å 90.00° 104.96° 90.00°	Depositor
Resolution (Å)	34.97 – 2.40 34.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.97-2.40) 99.6 (34.97-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.214 , 0.255 0.219 , 0.258	Depositor DCC
R_{free} test set	2552 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8734	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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	0.41	0/3599	0.52	0/4915
1	B	0.41	0/3609	0.53	0/4927
2	G	1.02	0/359	1.58	7/551 (1.3%)
2	I	0.80	0/381	1.19	1/585 (0.2%)
3	H	0.81	0/393	1.13	1/606 (0.2%)
3	J	0.63	0/393	1.03	1/606 (0.2%)
All	All	0.51	0/8734	0.72	10/12190 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	DT	O4'-C4'-C3'	-7.21	101.62	104.50
2	G	9	DT	N3-C4-O4	7.17	124.20	119.90
2	I	3	DT	O4'-C1'-N1	-6.74	103.28	108.00
2	G	9	DT	C5-C4-O4	-6.46	120.38	124.90
2	G	13	DA	O4'-C1'-N9	-6.25	103.63	108.00
3	J	6	DT	N3-C4-O4	5.90	123.44	119.90
2	G	5	DC	C6-N1-C2	5.65	122.56	120.30
3	H	11	DG	O4'-C1'-N9	5.34	111.74	108.00
2	G	1	DT	C6-C5-C7	-5.24	119.76	122.90
2	G	5	DC	O4'-C1'-N1	-5.05	104.47	108.00

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	3551	0	3708	137	1
1	B	3561	0	3718	131	2
2	G	321	0	182	3	0
2	I	341	0	194	10	1
3	H	350	0	194	5	0
3	J	350	0	194	25	0
4	A	99	0	0	10	0
4	B	90	0	0	6	0
4	G	24	0	0	2	0
4	H	13	0	0	0	0
4	I	27	0	0	4	0
4	J	7	0	0	5	0
All	All	8734	0	8190	304	2

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)
3:J:2:DC:OP2	4:J:105:HOH:O	1.60	1.17
1:A:550:ARG:HH12	1:A:551:LEU:CD2	1.62	1.11
1:A:550:ARG:HH12	1:A:551:LEU:CG	1.64	1.09
1:A:550:ARG:NH1	1:A:551:LEU:CD2	2.21	1.03
1:A:550:ARG:NH1	1:A:550:ARG:HG2	1.57	1.02
1:A:550:ARG:HH11	1:A:550:ARG:CG	1.71	1.02
1:A:523:GLN:OE1	1:A:524:ALA:HB2	1.63	0.96
1:B:417:PRO:O	1:B:421:GLN:HG3	1.66	0.95
1:B:687:GLN:NE2	1:B:695:LEU:HB2	1.81	0.94
1:A:550:ARG:HH12	1:A:551:LEU:HD21	1.32	0.94
1:B:249:ARG:NH2	1:B:257:THR:OG1	2.01	0.94
1:B:523:GLN:HA	1:B:523:GLN:NE2	1.81	0.93
1:A:722:GLU:O	4:A:870:HOH:O	1.89	0.91
1:A:550:ARG:NH1	1:A:551:LEU:HG	1.86	0.90
1:A:550:ARG:NH1	1:A:551:LEU:HD21	1.83	0.90
2:I:15:DA:N1	3:J:1:DT:N3	2.19	0.89
1:A:527:LEU:HD23	1:A:531:GLN:OE1	1.72	0.89
1:A:550:ARG:HH12	1:A:551:LEU:HG	1.36	0.88
3:J:-1:DA:H1'	3:J:0:DG:C8	2.11	0.86
1:A:550:ARG:NH1	1:A:551:LEU:CG	2.38	0.86
1:A:550:ARG:HG2	1:A:550:ARG:HH11	0.77	0.86
3:J:0:DG:H1'	3:J:1:DT:H5'	1.56	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLN:HB3	1:B:474:LYS:HD2	1.61	0.81
1:A:472:GLY:N	4:A:883:HOH:O	1.87	0.80
1:B:376:GLU:OE1	4:B:818:HOH:O	1.99	0.79
1:A:523:GLN:OE1	1:A:524:ALA:CB	2.30	0.79
1:B:687:GLN:NE2	1:B:692:ASP:H	1.80	0.78
1:A:619:LEU:HD21	1:A:651:GLN:OE1	1.81	0.78
3:J:-1:DA:H2"	3:J:0:DG:OP2	1.80	0.77
1:B:249:ARG:HH22	1:B:257:THR:HG1	1.32	0.77
1:A:522:CYS:SG	1:A:527:LEU:O	2.41	0.77
3:H:0:DG:H2"	3:H:1:DT:H5'	1.65	0.77
1:B:255:LEU:CD2	1:B:259:GLN:HB3	2.15	0.76
1:B:270:THR:OG1	4:B:828:HOH:O	2.04	0.76
1:B:694:ALA:C	1:B:695:LEU:HD23	2.07	0.75
1:A:516:ARG:HG2	1:A:517:LEU:HD13	1.69	0.74
1:B:546:GLU:OE1	4:B:829:HOH:O	2.04	0.74
2:I:5:DC:OP2	4:I:107:HOH:O	2.05	0.74
1:B:255:LEU:HD23	1:B:259:GLN:HB3	1.71	0.72
1:B:255:LEU:HD23	1:B:259:GLN:CB	2.19	0.72
1:A:536:ALA:HB2	1:A:545:LEU:HD11	1.70	0.72
1:B:252:PRO:HD2	1:B:279:ARG:HG2	1.72	0.71
1:B:440:LYS:HE2	4:G:116:HOH:O	1.90	0.71
1:A:661:HIS:CE1	1:A:688:LEU:O	2.44	0.70
1:B:523:GLN:HA	1:B:523:GLN:HE21	1.55	0.70
1:A:659:GLN:C	1:A:659:GLN:OE1	2.30	0.70
1:B:695:LEU:HD21	1:B:719:LYS:HG2	1.72	0.69
1:A:527:LEU:CD2	1:A:531:GLN:OE1	2.40	0.69
1:A:450:LEU:HD13	1:A:464:VAL:HG11	1.74	0.69
1:A:721:LEU:O	1:A:722:GLU:HB2	1.91	0.69
1:B:290:THR:OG1	1:B:293:GLN:HG3	1.93	0.68
1:B:577:GLN:HB3	1:B:610:LYS:HD3	1.76	0.68
1:B:586:LEU:HB3	1:B:587:PRO:HD3	1.76	0.67
1:A:586:LEU:N	1:A:587:PRO:HD2	2.08	0.67
1:A:712:ARG:HB3	1:A:713:PRO:HD3	1.77	0.67
1:A:448:ARG:O	1:A:451:PRO:HD2	1.93	0.67
1:B:518:LEU:HB3	1:B:519:PRO:HD3	1.77	0.66
1:A:535:ILE:HD11	1:A:567:VAL:HG23	1.78	0.66
1:A:276:HIS:O	1:A:279:ARG:HD2	1.96	0.65
1:A:586:LEU:O	1:A:590:CYS:SG	2.52	0.65
1:A:524:ALA:O	1:A:525:HIS:ND1	2.30	0.65
2:I:3:DT:OP2	4:I:109:HOH:O	2.14	0.65
1:A:550:ARG:NH1	1:A:550:ARG:CG	2.42	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:GLN:OE1	1:A:660:ALA:N	2.30	0.65
1:A:496:GLN:HB3	4:A:862:HOH:O	1.97	0.65
1:A:484:LEU:N	1:A:485:PRO:HD2	2.12	0.65
1:B:644:LYS:O	1:B:648:GLU:HG3	1.97	0.64
1:B:693:PRO:O	1:B:695:LEU:N	2.30	0.64
2:I:16:DC:H2"	2:I:17:DT:C6	2.33	0.64
1:A:651:GLN:O	1:A:651:GLN:HG3	1.96	0.64
1:A:570:ALA:HB2	1:A:579:LEU:HD11	1.80	0.64
1:B:672:ALA:HB2	1:B:681:LEU:HD11	1.80	0.63
1:A:658:CYS:O	1:A:662:GLY:HA2	1.99	0.63
1:A:543:GLN:HB3	1:A:576:LYS:HD3	1.81	0.63
1:A:516:ARG:HG2	1:A:517:LEU:CD1	2.29	0.62
1:B:586:LEU:HD13	1:B:600:VAL:HG11	1.81	0.62
3:J:0:DG:H2"	3:J:1:DT:OP2	2.00	0.61
1:A:659:GLN:OE1	1:A:660:ALA:HA	2.00	0.61
1:B:547:THR:OG1	1:B:576:LYS:HG3	2.00	0.61
1:B:434:ALA:HB2	1:B:443:LEU:HD11	1.82	0.61
1:B:445:THR:OG1	1:B:474:LYS:HG3	2.01	0.61
1:B:683:SER:HB3	1:B:715:LEU:HD12	1.83	0.61
1:B:305:GLN:HB3	1:B:338:LYS:HD2	1.83	0.60
1:B:584:ARG:HG2	1:B:585:LEU:HD13	1.82	0.60
1:B:518:LEU:HD13	1:B:532:VAL:HG11	1.82	0.60
1:A:521:LEU:HD21	1:A:549:GLN:HB2	1.84	0.60
1:B:695:LEU:HD23	1:B:695:LEU:N	2.17	0.59
1:B:689:SER:C	1:B:691:PRO:HD3	2.22	0.59
1:B:417:PRO:O	1:B:421:GLN:CG	2.47	0.59
1:B:407:GLN:HB3	1:B:440:LYS:HD3	1.83	0.59
2:G:1:DT:H6	2:G:1:DT:H5'	1.68	0.59
3:J:0:DG:H1'	3:J:1:DT:C5'	2.31	0.59
1:A:645:GLN:HB3	1:A:678:ARG:HD3	1.84	0.58
1:A:270:THR:CG2	1:A:304:LYS:HD2	2.33	0.58
1:A:564:GLN:O	1:A:567:VAL:HG12	2.03	0.58
1:B:411:THR:OG1	1:B:440:LYS:HG3	2.03	0.58
1:A:488:CYS:HA	1:A:493:LEU:O	2.03	0.58
1:B:479:THR:OG1	1:B:508:LYS:HG3	2.04	0.57
3:J:6:DT:OP1	4:J:101:HOH:O	2.17	0.57
1:B:523:GLN:NE2	1:B:523:GLN:CA	2.64	0.57
1:A:494:THR:HG21	4:A:862:HOH:O	2.05	0.57
1:A:345:GLN:NE2	4:A:830:HOH:O	2.37	0.57
3:J:14:DC:H2"	3:J:15:DA:C8	2.40	0.57
1:A:567:VAL:O	1:A:571:SER:OG	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HD21	1:A:586:LEU:HD11	1.87	0.56
1:B:552:LEU:HB3	1:B:553:PRO:HD3	1.85	0.56
1:B:450:LEU:HB3	1:B:451:PRO:HD3	1.88	0.56
1:A:516:ARG:HE	1:A:517:LEU:HD13	1.70	0.56
1:B:248:LEU:HD21	1:B:276:HIS:HA	1.87	0.56
1:B:487:LEU:HD21	1:B:515:GLN:HB2	1.87	0.56
1:A:661:HIS:HE1	1:A:688:LEU:O	1.86	0.56
1:A:574:GLY:N	4:A:807:HOH:O	2.30	0.55
1:A:368:ASN:HB2	4:A:880:HOH:O	2.05	0.55
3:J:-1:DA:H1'	3:J:0:DG:N7	2.22	0.55
1:B:245:ALA:O	1:B:249:ARG:HG3	2.07	0.55
1:A:649:THR:HG22	1:A:653:LEU:HD12	1.89	0.55
3:J:2:DC:P	4:J:105:HOH:O	2.51	0.55
1:B:378:VAL:O	1:B:382:LEU:HB2	2.06	0.55
1:B:692:ASP:O	1:B:693:PRO:C	2.45	0.55
1:B:408:ALA:O	1:B:412:VAL:HG23	2.08	0.54
2:G:13:DA:OP2	4:G:110:HOH:O	2.18	0.54
1:A:620:LEU:HD12	1:A:620:LEU:O	2.06	0.54
1:A:721:LEU:O	1:A:722:GLU:CB	2.55	0.54
1:B:663:LEU:HD11	1:B:688:LEU:HD21	1.90	0.54
1:B:496:GLN:H	1:B:496:GLN:CD	2.11	0.54
1:B:715:LEU:O	1:B:719:LYS:HG3	2.08	0.54
1:A:659:GLN:OE1	1:A:660:ALA:CA	2.55	0.53
1:B:678:ARG:CB	1:B:679:PRO:CD	2.86	0.53
1:A:552:LEU:N	1:A:553:PRO:HD2	2.23	0.53
2:I:16:DC:H2"	2:I:17:DT:H5"	1.91	0.53
1:A:372:LYS:O	1:A:376:GLU:HG3	2.08	0.53
1:A:516:ARG:HG2	1:A:516:ARG:O	2.08	0.53
3:J:3:DT:H4'	4:J:107:HOH:O	2.08	0.53
1:B:306:ALA:O	1:B:310:VAL:HG13	2.08	0.53
1:B:309:THR:OG1	1:B:338:LYS:HG3	2.09	0.53
1:A:586:LEU:N	1:A:587:PRO:CD	2.72	0.53
1:B:667:GLN:HG2	1:B:704:VAL:HG11	1.90	0.53
1:B:250:GLY:O	1:B:254:GLN:N	2.36	0.53
1:B:596:THR:HG22	1:B:597:PRO:HD2	1.90	0.53
1:A:373:GLN:HB3	1:A:406:LYS:HD3	1.90	0.52
1:B:690:ARG:O	1:B:691:PRO:C	2.48	0.52
1:B:717:ALA:O	1:B:721:LEU:HD12	2.08	0.52
1:B:433:ILE:HD13	1:B:446:VAL:HG21	1.90	0.52
1:B:687:GLN:HE21	1:B:695:LEU:HB2	1.67	0.52
1:A:252:PRO:HD2	1:A:279:ARG:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:ARG:HB3	1:B:679:PRO:CD	2.39	0.52
1:A:658:CYS:HA	1:A:663:LEU:H	1.75	0.52
1:B:253:LEU:HD23	1:B:279:ARG:HG3	1.91	0.52
1:B:588:VAL:O	1:B:592:ALA:N	2.35	0.52
1:B:518:LEU:HB3	1:B:519:PRO:CD	2.40	0.52
1:B:681:LEU:O	1:B:684:ILE:HG22	2.10	0.51
3:J:0:DG:OP2	3:J:0:DG:H8	1.93	0.51
1:B:687:GLN:O	1:B:691:PRO:HA	2.10	0.51
3:J:0:DG:C1'	3:J:1:DT:H5'	2.35	0.51
1:B:352:CYS:HA	1:B:357:LEU:O	2.10	0.51
1:B:531:GLN:O	1:B:535:ILE:HG13	2.10	0.51
1:A:550:ARG:O	1:A:551:LEU:HD23	2.11	0.51
1:A:416:LEU:N	1:A:417:PRO:HD2	2.25	0.51
1:A:562:THR:O	1:A:565:GLN:N	2.44	0.50
1:A:491:HIS:HB3	1:A:518:LEU:HD22	1.93	0.50
1:A:658:CYS:SG	1:A:663:LEU:O	2.68	0.50
1:B:343:THR:O	1:B:347:LEU:HB2	2.11	0.50
1:B:249:ARG:O	1:B:254:GLN:HA	2.10	0.50
1:A:521:LEU:HD23	1:A:525:HIS:HD2	1.76	0.50
1:B:241:LEU:O	1:B:245:ALA:HB2	2.11	0.50
1:B:616:VAL:O	1:B:620:LEU:HB2	2.12	0.50
1:B:620:LEU:N	1:B:621:PRO:CD	2.75	0.50
1:B:300:HIS:HB3	1:B:335:ASP:OD1	2.12	0.50
1:B:668:VAL:HG13	1:B:681:LEU:HD21	1.93	0.50
1:A:715:LEU:O	1:A:718:VAL:HG12	2.11	0.49
1:B:479:THR:O	1:B:483:LEU:HB2	2.11	0.49
1:B:690:ARG:O	1:B:691:PRO:O	2.30	0.49
1:A:516:ARG:O	1:A:516:ARG:CG	2.61	0.49
1:B:700:ASN:OD1	4:B:837:HOH:O	2.19	0.49
1:A:474:LYS:O	1:A:478:GLU:HG3	2.13	0.49
1:B:266:ARG:HH12	3:H:9:DT:H2'	1.77	0.49
1:B:661:HIS:CD2	1:B:688:LEU:HB3	2.48	0.49
1:B:412:VAL:O	1:B:416:LEU:HB2	2.13	0.49
1:B:427:PRO:HD2	1:B:428:GLN:OE1	2.12	0.48
1:A:265:LYS:HE2	3:J:9:DT:OP1	2.12	0.48
1:B:370:GLY:N	4:B:875:HOH:O	2.44	0.48
1:A:293:GLN:O	1:A:297:ILE:HG13	2.13	0.48
1:A:382:LEU:O	1:A:382:LEU:HD23	2.13	0.48
1:B:495:PRO:HB2	1:B:496:GLN:OE1	2.14	0.48
3:H:-1:DA:H2"	3:H:0:DG:OP2	2.13	0.48
1:A:646:ALA:O	1:A:650:VAL:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ARG:N	1:A:679:PRO:HD2	2.29	0.48
1:B:620:LEU:N	1:B:621:PRO:HD2	2.29	0.48
1:A:518:LEU:HB3	1:A:519:PRO:HD3	1.95	0.48
1:A:620:LEU:HB3	1:A:621:PRO:HD3	1.96	0.48
1:B:603:ILE:HD13	1:B:616:VAL:HG21	1.96	0.48
1:B:693:PRO:C	1:B:695:LEU:N	2.67	0.47
1:A:297:ILE:HD13	1:A:310:VAL:HG21	1.96	0.47
1:A:359:PRO:O	1:A:363:VAL:HG23	2.13	0.47
1:A:416:LEU:HD12	1:A:416:LEU:O	2.14	0.47
1:B:654:LEU:HD13	1:B:668:VAL:HG11	1.97	0.47
1:B:693:PRO:O	1:B:696:ALA:N	2.48	0.47
2:I:1:DT:H2"	2:I:2:DG:H8	1.78	0.47
1:B:249:ARG:NH2	1:B:257:THR:N	2.63	0.47
1:A:672:ALA:HB2	1:A:681:LEU:HD11	1.96	0.47
1:A:414:ARG:NH1	4:A:815:HOH:O	2.47	0.47
1:A:709:LEU:C	1:A:709:LEU:HD23	2.35	0.47
1:B:352:CYS:SG	1:B:357:LEU:O	2.72	0.47
1:B:252:PRO:CD	1:B:279:ARG:HG2	2.43	0.47
3:J:3:DT:C4'	4:J:107:HOH:O	2.63	0.47
1:A:516:ARG:HE	1:A:517:LEU:CD1	2.28	0.47
1:B:501:ILE:O	4:B:803:HOH:O	2.20	0.47
1:A:251:PRO:HA	1:A:252:PRO:HA	1.68	0.46
1:B:302:GLY:O	1:B:303:GLY:C	2.54	0.46
2:I:15:DA:N3	4:I:111:HOH:O	2.35	0.46
1:B:671:ILE:HG23	1:B:707:ALA:HB1	1.98	0.46
1:A:484:LEU:N	1:A:485:PRO:CD	2.78	0.46
1:A:561:LEU:HA	1:A:565:GLN:OE1	2.15	0.46
1:A:603:ILE:HD13	1:A:616:VAL:HG21	1.98	0.46
2:I:4:DC:H2"	2:I:5:DC:O5'	2.15	0.46
1:B:253:LEU:HD23	1:B:279:ARG:CG	2.46	0.46
1:B:550:ARG:NH2	1:B:580:GLU:OE2	2.48	0.46
1:A:638:ALA:HB2	1:A:647:LEU:HD11	1.96	0.46
3:J:8:DG:H1'	3:J:9:DT:H5'	1.96	0.46
1:B:399:ILE:HD13	1:B:412:VAL:HG21	1.98	0.46
1:A:661:HIS:ND1	1:A:688:LEU:HB3	2.31	0.46
1:B:509:GLN:HB3	1:B:542:LYS:HD3	1.98	0.46
1:A:627:HIS:HB3	1:A:654:LEU:CD2	2.46	0.46
1:A:561:LEU:HD11	1:A:586:LEU:HD11	1.98	0.46
1:A:486:VAL:C	1:A:487:LEU:HD23	2.37	0.45
1:B:508:LYS:O	1:B:512:GLU:HG3	2.16	0.45
1:A:506:GLY:N	4:A:885:HOH:O	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:THR:O	1:A:634:VAL:HG23	2.16	0.45
3:J:1:DT:H2"	3:J:2:DC:C6	2.51	0.45
1:B:310:VAL:HG12	1:B:341:LEU:HD11	1.97	0.45
1:B:657:LEU:HD13	1:B:668:VAL:HG22	1.99	0.45
1:B:392:THR:OG1	1:B:395:GLN:HG3	2.17	0.45
1:A:314:LEU:HD23	1:A:314:LEU:C	2.36	0.45
1:A:318:CYS:HA	1:A:323:LEU:O	2.18	0.44
1:A:523:GLN:OE1	1:A:524:ALA:N	2.50	0.44
2:I:1:DT:H2"	2:I:2:DG:C8	2.52	0.44
1:A:654:LEU:HB3	1:A:655:PRO:HD3	1.97	0.44
1:B:278:TRP:CH2	1:B:308:GLU:HB2	2.52	0.44
1:B:348:LEU:HB3	1:B:349:PRO:HD3	1.99	0.44
1:A:472:GLY:CA	4:A:883:HOH:O	2.49	0.44
1:B:665:PRO:HB2	1:B:666:GLN:NE2	2.32	0.44
1:B:654:LEU:N	1:B:655:PRO:CD	2.81	0.44
1:A:266:ARG:NH1	3:J:9:DT:OP2	2.40	0.44
1:A:382:LEU:N	1:A:383:PRO:CD	2.81	0.44
1:B:693:PRO:O	1:B:694:ALA:C	2.57	0.44
1:A:243:THR:O	1:A:247:GLU:HG3	2.18	0.43
1:A:438:GLY:N	4:I:119:HOH:O	2.43	0.43
3:J:-1:DA:C2'	3:J:0:DG:OP2	2.59	0.43
1:B:666:GLN:H	1:B:666:GLN:CD	2.22	0.43
1:B:678:ARG:HB3	1:B:679:PRO:HD3	2.00	0.43
1:A:265:LYS:CE	3:J:9:DT:OP1	2.67	0.42
1:A:270:THR:HG22	1:A:304:LYS:HD2	2.00	0.42
1:A:532:VAL:HA	1:A:535:ILE:HD12	2.01	0.42
1:A:450:LEU:HD12	1:A:450:LEU:O	2.19	0.42
1:B:596:THR:H	1:B:596:THR:HG1	1.43	0.42
1:A:305:GLN:HB3	1:A:338:LYS:HD2	2.01	0.42
1:A:338:LYS:O	1:A:342:GLU:HG3	2.19	0.42
1:A:487:LEU:HB3	1:A:493:LEU:HD12	2.01	0.42
1:B:695:LEU:O	1:B:697:ALA:N	2.52	0.42
1:A:325:PRO:O	1:A:329:VAL:HG23	2.19	0.42
1:A:407:GLN:HB3	1:A:440:LYS:HD3	2.01	0.42
3:J:-1:DA:C4	3:J:0:DG:C6	3.07	0.42
1:B:321:HIS:CD2	1:B:348:LEU:HD22	2.55	0.42
1:A:352:CYS:HA	1:A:357:LEU:O	2.20	0.42
2:I:16:DC:H2"	2:I:17:DT:H6	1.81	0.42
1:B:353:GLN:HE21	1:B:353:GLN:HB2	1.58	0.42
1:B:615:THR:OG1	1:B:644:LYS:HG3	2.19	0.42
1:A:559:HIS:HB3	1:A:586:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:O	1:A:389:HIS:HB2	2.19	0.41
1:A:516:ARG:O	1:A:517:LEU:HD12	2.19	0.41
1:A:552:LEU:N	1:A:553:PRO:CD	2.83	0.41
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.89	0.41
3:J:0:DG:C2'	3:J:1:DT:OP2	2.68	0.41
1:B:468:ALA:HB2	1:B:477:LEU:HD11	2.03	0.41
1:B:559:HIS:HB3	1:B:586:LEU:HD23	2.02	0.41
1:A:611:GLN:O	1:A:644:LYS:HB2	2.20	0.41
1:A:702:HIS:HB3	1:B:702:HIS:CE1	2.55	0.41
1:B:480:VAL:HG22	1:B:511:LEU:HD11	2.03	0.41
1:A:392:THR:OG1	1:A:395:GLN:HG3	2.20	0.41
1:B:256:ASP:O	1:B:260:LEU:HD22	2.21	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.82	0.41
1:B:249:ARG:NH2	1:B:257:THR:CA	2.84	0.41
1:B:347:LEU:HA	1:B:347:LEU:HD12	1.84	0.41
3:J:14:DC:H2"	3:J:15:DA:O5'	2.20	0.41
1:B:267:GLY:HA2	1:B:300:HIS:O	2.21	0.41
1:B:276:HIS:O	1:B:279:ARG:HB2	2.20	0.41
1:B:633:GLN:O	1:B:637:ILE:HG13	2.20	0.41
2:G:10:DA:C2	3:H:7:DA:C2	3.09	0.41
1:A:494:THR:O	1:A:497:GLN:N	2.46	0.41
1:A:254:GLN:HE21	1:A:254:GLN:HB2	1.73	0.40
1:A:314:LEU:HB3	1:A:315:PRO:HD3	2.02	0.40
1:A:491:HIS:CD2	1:A:518:LEU:HD22	2.56	0.40
1:A:537:SER:O	1:A:538:HIS:CG	2.74	0.40
1:B:406:LYS:O	1:B:410:GLU:HG3	2.21	0.40
1:A:266:ARG:HA	1:A:266:ARG:NE	2.37	0.40
1:A:463:GLN:O	1:A:467:ILE:HG13	2.22	0.40
3:J:0:DG:C8	3:J:0:DG:OP2	2.72	0.40
1:A:720:LYS:HE3	1:A:720:LYS:HB2	1.88	0.40
3:H:0:DG:C2'	3:H:1:DT:H5'	2.44	0.40
1:B:307:LEU:O	1:B:311:GLN:HG3	2.22	0.40
1:B:682:GLU:O	1:B:685:VAL:HG12	2.22	0.40
1:A:287:LEU:HD22	1:A:287:LEU:HA	1.92	0.40
1:A:445:THR:OG1	1:A:474:LYS:HB2	2.21	0.40
1:B:460:THR:OG1	1:B:463:GLN:HG3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:SER:N	1:B:232:TRP:O[1_656]	2.10	0.10
2:I:1:DT:O5'	1:B:233:SER:OG[1_656]	2.15	0.05

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	489/499 (98%)	454 (93%)	33 (7%)	2 (0%)	34 48
1	B	487/499 (98%)	442 (91%)	36 (7%)	9 (2%)	8 10
All	All	976/998 (98%)	896 (92%)	69 (7%)	11 (1%)	14 20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	691	PRO
1	B	694	ALA
1	A	553	PRO
1	B	486	VAL
1	B	693	PRO
1	B	696	ALA
1	A	485	PRO
1	B	303	GLY
1	B	279	ARG
1	B	519	PRO
1	B	587	PRO

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	379/387 (98%)	343 (90%)	36 (10%)	8 12
1	B	380/387 (98%)	348 (92%)	32 (8%)	11 16
All	All	759/774 (98%)	691 (91%)	68 (9%)	9 14

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	A	254	GLN
1	A	262	LYS
1	A	279	ARG
1	A	287	LEU
1	A	316	VAL
1	A	319	GLN
1	A	345	GLN
1	A	387	GLN
1	A	453	LEU
1	A	455	GLN
1	A	459	LEU
1	A	460	THR
1	A	486	VAL
1	A	494	THR
1	A	516	ARG
1	A	523	GLN
1	A	528	THR
1	A	550	ARG
1	A	557	GLN
1	A	561	LEU
1	A	583	GLN
1	A	586	LEU
1	A	591	GLN
1	A	623	LEU
1	A	625	GLN
1	A	632	GLU
1	A	651	GLN
1	A	659	GLN
1	A	663	LEU
1	A	666	GLN
1	A	684	ILE
1	A	687	GLN
1	A	689	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	706	LEU
1	A	718	VAL
1	B	231	GLN
1	B	236	ARG
1	B	238	LEU
1	B	249	ARG
1	B	255	LEU
1	B	260	LEU
1	B	266	ARG
1	B	270	THR
1	B	292	GLU
1	B	346	ARG
1	B	350	VAL
1	B	351	LEU
1	B	382	LEU
1	B	416	LEU
1	B	421	GLN
1	B	428	GLN
1	B	455	GLN
1	B	482	ARG
1	B	520	VAL
1	B	523	GLN
1	B	585	LEU
1	B	596	THR
1	B	598	GLU
1	B	607	SER
1	B	620	LEU
1	B	622	VAL
1	B	688	LEU
1	B	689	SER
1	B	695	LEU
1	B	702	HIS
1	B	718	VAL
1	B	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	345	GLN
1	A	591	GLN
1	A	593	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	640	ASN
1	A	661	HIS
1	B	231	GLN
1	B	276	HIS
1	B	334	HIS
1	B	353	GLN
1	B	421	GLN
1	B	436	HIS
1	B	457	HIS
1	B	523	GLN
1	B	666	GLN
1	B	687	GLN
1	B	702	HIS

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 monosaccharides 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	490/499 (98%)	0.26	19 (3%) 39 38	25, 51, 87, 128	9 (1%)
1	B	491/499 (98%)	0.32	14 (2%) 51 50	24, 49, 86, 114	8 (1%)
2	G	16/17 (94%)	-0.43	0 100 100	27, 33, 51, 70	0
2	I	17/17 (100%)	-0.04	1 (5%) 22 21	32, 40, 101, 146	0
3	H	17/17 (100%)	0.31	2 (11%) 4 4	20, 50, 86, 130	0
3	J	17/17 (100%)	0.53	2 (11%) 4 4	20, 51, 117, 134	0
All	All	1048/1066 (98%)	0.28	38 (3%) 42 42	20, 50, 87, 146	17 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	ALA	3.9
1	A	233	SER	3.8
2	I	17	DT	3.7
3	J	1	DT	3.7
1	A	557	GLN	3.4
1	A	525	HIS	3.4
1	B	695	LEU	3.4
1	B	654	LEU	3.1
1	A	522	CYS	3.1
1	B	492	GLY	3.0
1	B	251	PRO	2.9
1	A	690	ARG	2.8
1	B	696	ALA	2.7
1	B	523	GLN	2.7
1	A	662	GLY	2.7
1	A	553	PRO	2.5
3	H	-1	DA	2.5
1	A	493	LEU	2.5
1	B	593	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	625	GLN	2.4
1	A	551	LEU	2.3
1	A	559	HIS	2.3
3	H	1	DT	2.2
1	A	521	LEU	2.2
1	B	421	GLN	2.2
1	A	685	VAL	2.2
1	A	580	GLU	2.1
1	B	693	PRO	2.1
1	A	564	GLN	2.1
3	J	0	DG	2.1
1	B	557	GLN	2.1
1	B	720	LYS	2.1
1	A	563	PRO	2.1
1	B	692	ASP	2.0
1	A	558	ALA	2.0
1	A	387	GLN	2.0
1	B	721	LEU	2.0
1	A	548	VAL	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.