Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 07:00 PM EDT

PDB ID	:	4OSI
Title	:	Crystal structure of the TAL effector dHax3 with NI RVD at 2.8 angstrom resolution
Authors	:	Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.
Deposited on	:	2014-02-13
Resolution	:	2.85 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:

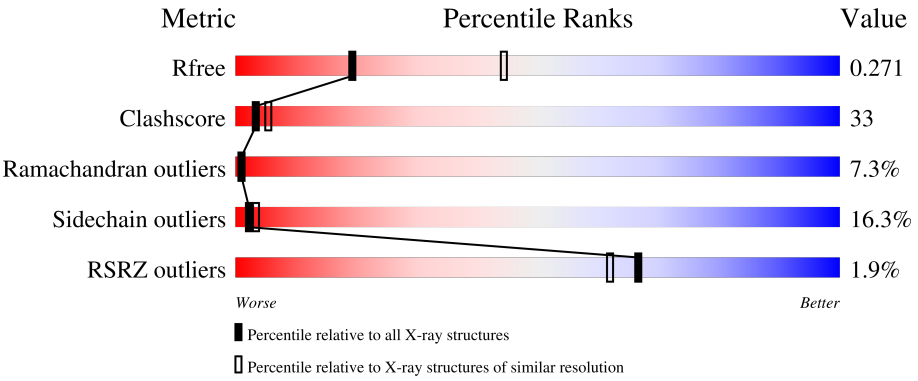
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.85 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	49% 40% 7%
1	B	499	3% 35% 46% 15%
2	G	17	35% 53% 12%
2	I	17	12% 35% 47% 6%
3	H	17	24% 71% 6%

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 8411 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	485	Total	C	N	O	S	4	1	0
			3509	2194	651	652	12			
1	B	486	Total	C	N	O	S	4	0	0
			3521	2202	655	652	12			

There are 54 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	368	HIS	ASN	engineered mutation	UNP Q3ZD72
A	369	ASP	ILE	engineered mutation	UNP Q3ZD72
A	402	ASN	HIS	engineered mutation	UNP Q3ZD72
A	403	GLY	ASP	engineered mutation	UNP Q3ZD72
A	436	ASN	HIS	engineered mutation	UNP Q3ZD72
A	437	GLY	ASP	engineered mutation	UNP Q3ZD72
A	470	ASN	HIS	engineered mutation	UNP Q3ZD72
A	471	GLY	ASP	engineered mutation	UNP Q3ZD72
A	505	ILE	SER	engineered mutation	UNP Q3ZD72
A	539	GLY	SER	engineered mutation	UNP Q3ZD72
A	572	HIS	ASN	engineered mutation	UNP Q3ZD72
A	573	ASP	SER	engineered mutation	UNP Q3ZD72
A	606	ASN	HIS	engineered mutation	UNP Q3ZD72
A	607	GLY	ASP	engineered mutation	UNP Q3ZD72
A	640	HIS	ASN	engineered mutation	UNP Q3ZD72
A	641	ASP	ILE	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
B	301	ASP	ILE	engineered mutation	UNP Q3ZD72
B	368	HIS	ASN	engineered mutation	UNP Q3ZD72
B	369	ASP	ILE	engineered mutation	UNP Q3ZD72
B	402	ASN	HIS	engineered mutation	UNP Q3ZD72
B	403	GLY	ASP	engineered mutation	UNP Q3ZD72
B	436	ASN	HIS	engineered mutation	UNP Q3ZD72
B	437	GLY	ASP	engineered mutation	UNP Q3ZD72
B	470	ASN	HIS	engineered mutation	UNP Q3ZD72
B	471	GLY	ASP	engineered mutation	UNP Q3ZD72
B	505	ILE	SER	engineered mutation	UNP Q3ZD72
B	539	GLY	SER	engineered mutation	UNP Q3ZD72
B	572	HIS	ASN	engineered mutation	UNP Q3ZD72
B	573	ASP	SER	engineered mutation	UNP Q3ZD72
B	606	ASN	HIS	engineered mutation	UNP Q3ZD72
B	607	GLY	ASP	engineered mutation	UNP Q3ZD72
B	640	HIS	ASN	engineered mutation	UNP Q3ZD72
B	641	ASP	ILE	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*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	16	Total	C	N	O	P	0	0	0
			316	153	44	103	16			
2	G	17	Total	C	N	O	P	0	0	0
			333	163	46	108	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	16	Total	C	N	O	P	0	0	0
			336	159	75	87	15			
3	H	17	Total	C	N	O	P	0	0	0
			357	169	80	92	16			

- Molecule 4 is water.

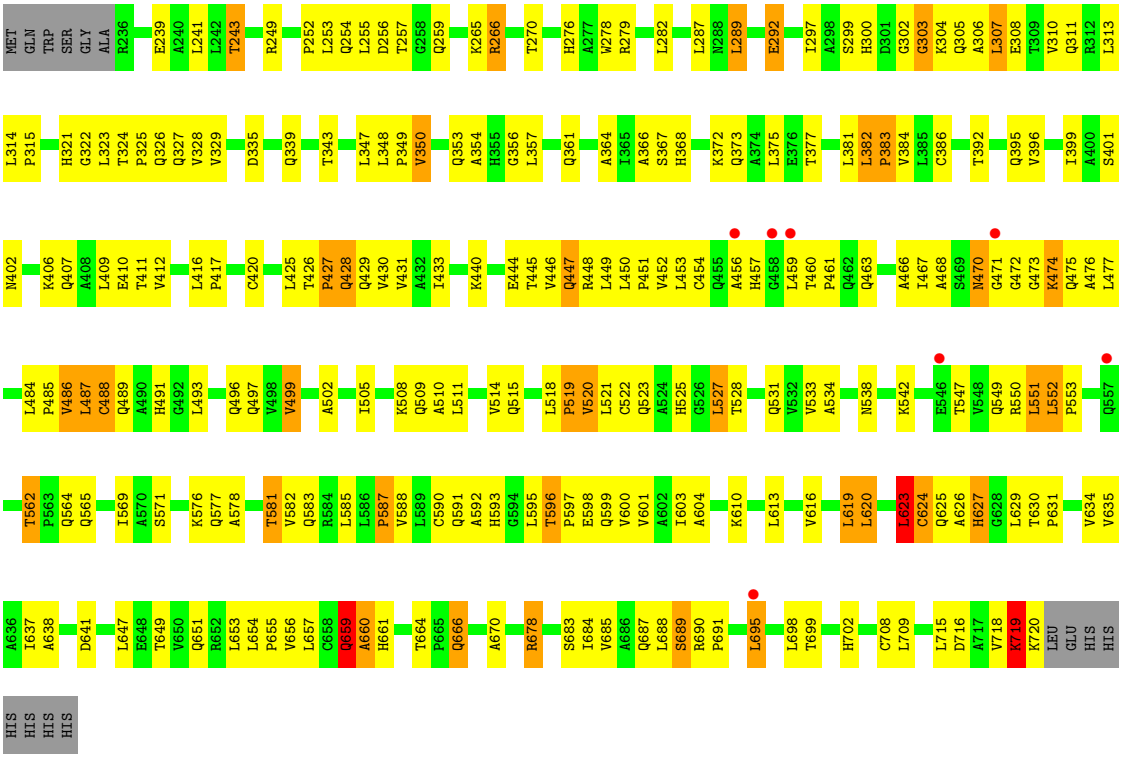
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	I	8	Total	O	0	0
			8	8		
4	B	9	Total	O	0	0
			9	9		
4	G	4	Total	O	0	0
			4	4		

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.

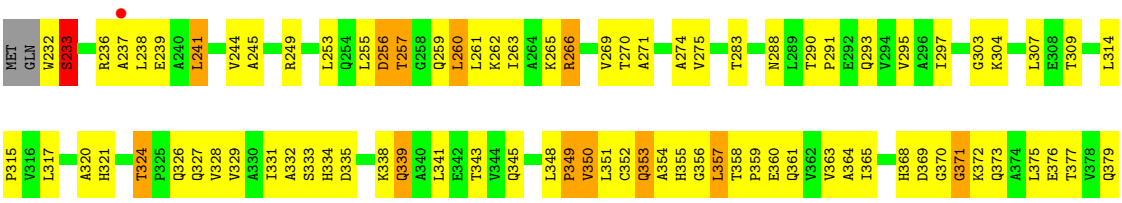
• Molecule 1: Hax3

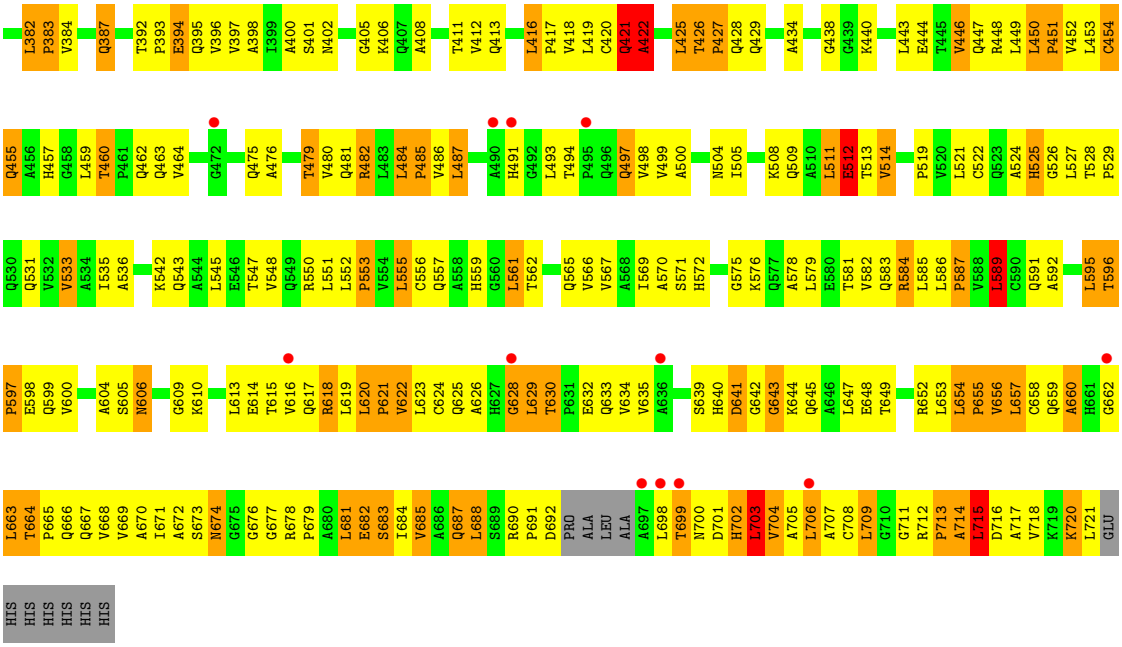
Chain A:



• Molecule 1: Hax3

Chain B:



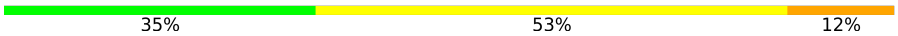


• Molecule 2: DNA (5’-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*CP*T)-3’)

Chain I:

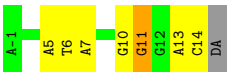
• Molecule 2: DNA (5’-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*CP*T)-3’)

Chain G:



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

Chain J:



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.29Å 89.36Å 90.27Å 90.00° 103.74° 90.00°	Depositor
Resolution (Å)	31.99 – 2.85 31.99 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (31.99-2.85) 99.4 (31.99-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.243 , 0.286 0.232 , 0.271	Depositor DCC
R_{free} test set	1532 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	75.6	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 37.2	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	0.94	EDS
Total number of atoms	8411	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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	0.48	0/3558	0.61	0/4860
1	B	0.46	0/3570	0.67	2/4873 (0.0%)
2	G	0.87	0/368	1.73	10/564 (1.8%)
2	I	0.91	0/349	2.08	17/534 (3.2%)
3	H	0.81	0/405	1.43	4/625 (0.6%)
3	J	0.91	0/381	1.61	6/588 (1.0%)
All	All	0.56	0/8631	0.95	39/12044 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	422	ALA	N-CA-CB	-14.25	90.16	110.10
1	B	422	ALA	N-CA-C	11.28	141.46	111.00
3	J	5	DA	O4'-C1'-N9	10.97	115.68	108.00
3	H	10	DG	O4'-C1'-N9	10.76	115.53	108.00
2	I	3	DT	O4'-C1'-C2'	-10.73	97.32	105.90
2	I	5	DC	O4'-C1'-N1	9.88	114.92	108.00
2	I	15	DT	O4'-C1'-N1	-9.50	101.35	108.00
3	J	6	DT	N3-C4-O4	9.25	125.45	119.90
2	G	8	DT	N3-C4-O4	8.38	124.92	119.90
3	H	4	DG	O4'-C1'-N9	8.06	113.64	108.00
2	G	3	DT	N3-C4-O4	8.04	124.72	119.90
3	J	11	DG	O4'-C1'-N9	8.00	113.60	108.00
2	I	2	DG	O4'-C1'-N9	7.97	113.58	108.00
3	J	6	DT	O4'-C1'-N1	7.36	113.15	108.00
2	I	3	DT	C1'-O4'-C4'	-7.05	103.05	110.10
3	J	6	DT	C5-C4-O4	-7.01	119.99	124.90
2	I	16	DC	O4'-C4'-C3'	-6.75	101.80	104.50
2	G	7	DT	O4'-C1'-N1	-6.56	103.41	108.00
2	I	4	DC	O4'-C1'-C2'	-6.09	101.03	105.90
2	G	3	DT	C5-C4-O4	-6.05	120.66	124.90
3	H	7	DA	O4'-C1'-N9	6.05	112.24	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	13	DT	N3-C4-O4	6.02	123.51	119.90
2	G	8	DT	C5-C4-O4	-5.93	120.75	124.90
2	G	11	DT	N3-C4-O4	5.89	123.44	119.90
2	G	6	DC	O4'-C1'-N1	-5.81	103.93	108.00
2	I	8	DT	C5-C4-O4	-5.72	120.89	124.90
2	I	13	DT	O4'-C4'-C3'	-5.70	102.22	104.50
2	I	2	DG	O4'-C1'-C2'	-5.48	101.52	105.90
2	I	4	DC	O4'-C1'-N1	5.45	111.81	108.00
3	J	7	DA	C8-N9-C4	5.42	107.97	105.80
2	G	11	DT	C5-C4-O4	-5.39	121.13	124.90
2	I	4	DC	C1'-O4'-C4'	-5.38	104.72	110.10
2	I	11	DT	C5-C4-O4	-5.15	121.29	124.90
2	I	3	DT	C4-C5-C7	5.14	122.09	119.00
2	I	9	DT	N3-C4-O4	5.09	122.95	119.90
2	I	8	DT	N3-C4-O4	5.07	122.94	119.90
2	G	13	DT	C5-C4-O4	-5.02	121.39	124.90
2	I	13	DT	O4'-C1'-N1	-5.01	104.49	108.00
3	H	8	DA	O4'-C1'-N9	5.01	111.50	108.00

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	3509	0	3664	197	0
1	B	3521	0	3676	308	1
2	G	333	0	195	11	0
2	I	316	0	182	11	0
3	H	357	0	190	14	0
3	J	336	0	179	3	0
4	A	18	0	0	1	0
4	B	9	0	0	0	0
4	G	4	0	0	1	0
4	I	8	0	0	3	0
All	All	8411	0	8086	537	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (537) 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:249:ARG:NH2	1:B:257:THR:HG23	1.42	1.35
1:B:553:PRO:O	1:B:557:GLN:HG3	1.30	1.32
1:B:265:LYS:HE2	1:B:266:ARG:NH2	1.44	1.28
1:B:265:LYS:CE	1:B:266:ARG:NH2	2.02	1.23
1:B:265:LYS:CE	1:B:266:ARG:HH22	1.52	1.22
1:B:255:LEU:HD23	1:B:259:GLN:OE1	1.42	1.18
1:B:350:VAL:O	1:B:354:ALA:HB3	1.43	1.18
1:B:249:ARG:HH22	1:B:257:THR:CG2	1.59	1.13
1:B:553:PRO:O	1:B:557:GLN:CG	2.02	1.07
1:B:351:LEU:O	1:B:357:LEU:HB2	1.58	1.04
1:B:493:LEU:HB3	1:B:497:GLN:OE1	1.58	1.03
1:B:714:ALA:O	1:B:717:ALA:N	1.92	1.03
1:B:249:ARG:HH22	1:B:257:THR:HG23	0.86	1.02
1:B:357:LEU:HD23	1:B:361:GLN:OE1	1.58	1.01
2:G:14:DC:H2"	2:G:15:DT:H5"	1.42	1.01
1:B:357:LEU:CD2	1:B:361:GLN:OE1	2.13	0.97
1:B:425:LEU:HD12	1:B:429:GLN:OE1	1.65	0.96
1:B:350:VAL:O	1:B:354:ALA:CB	2.17	0.92
1:B:265:LYS:HE2	1:B:266:ARG:HH22	1.06	0.91
1:A:655:PRO:O	1:A:659:GLN:HG2	1.70	0.91
1:A:287:LEU:HD11	1:A:311:GLN:HA	1.54	0.89
1:B:555:LEU:HD21	1:B:583:GLN:HB2	1.54	0.89
1:B:453:LEU:HB3	1:B:459:LEU:HD12	1.54	0.88
1:B:348:LEU:HD13	1:B:352:CYS:SG	2.14	0.88
1:B:265:LYS:HE3	1:B:266:ARG:NH2	1.87	0.88
1:B:256:ASP:O	1:B:260:LEU:HD22	1.74	0.88
1:A:373:GLN:HB3	1:A:406:LYS:HD2	1.56	0.87
1:B:720:LYS:O	1:B:721:LEU:HG	1.74	0.87
1:B:715:LEU:HD23	1:B:715:LEU:H	1.41	0.85
1:B:493:LEU:CB	1:B:497:GLN:OE1	2.25	0.83
1:B:715:LEU:O	1:B:718:VAL:N	2.11	0.83
1:A:484:LEU:O	1:A:488:CYS:HB2	1.78	0.83
1:B:656:VAL:O	1:B:660:ALA:HB3	1.78	0.82
1:A:661:HIS:CD2	1:A:688:LEU:HB3	2.15	0.81
1:A:491:HIS:HB3	1:A:518:LEU:CD2	2.12	0.80
1:A:587:PRO:O	1:A:591:GLN:NE2	2.14	0.80
1:B:720:LYS:O	1:B:721:LEU:CD2	2.30	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:LYS:O	1:B:721:LEU:CG	2.30	0.79
1:B:720:LYS:C	1:B:721:LEU:HG	2.02	0.79
1:B:712:ARG:NH2	2:G:15:DT:OP1	2.16	0.79
2:I:9:DT:OP2	4:I:104:HOH:O	2.00	0.79
1:A:491:HIS:HB3	1:A:518:LEU:HD23	1.65	0.78
1:A:292:GLU:CD	1:A:292:GLU:H	1.84	0.78
1:A:425:LEU:HD21	1:A:450:LEU:HD21	1.65	0.78
1:B:249:ARG:NH2	1:B:257:THR:CG2	2.28	0.78
1:B:711:GLY:C	1:B:713:PRO:HD2	2.04	0.78
1:B:644:LYS:HE3	1:B:648:GLU:OE2	1.83	0.77
1:B:487:LEU:O	1:B:493:LEU:N	2.17	0.77
1:A:306:ALA:O	1:A:310:VAL:HG23	1.85	0.76
2:G:13:DT:H2"	2:G:14:DC:H5"	1.66	0.76
1:B:720:LYS:O	1:B:721:LEU:HD23	1.86	0.76
1:A:599:GLN:O	1:A:603:ILE:HG13	1.86	0.75
1:B:339:GLN:HG3	1:B:372:LYS:HD3	1.68	0.75
1:A:395:GLN:O	1:A:399:ILE:HD12	1.85	0.75
1:B:543:GLN:HB3	1:B:576:LYS:HD3	1.68	0.75
1:B:255:LEU:CD2	1:B:259:GLN:OE1	2.30	0.74
1:B:349:PRO:O	1:B:353:GLN:HG2	1.87	0.74
1:A:282:LEU:HD21	1:A:311:GLN:HG3	1.70	0.74
1:A:502:ALA:HB2	1:A:511:LEU:HD11	1.69	0.74
1:B:382:LEU:HD23	1:B:396:VAL:HG11	1.69	0.74
1:A:468:ALA:HB2	1:A:477:LEU:HD11	1.69	0.74
1:A:366:ALA:HB2	1:A:375:LEU:HD11	1.68	0.73
1:B:377:THR:OG1	1:B:406:LYS:HG3	1.88	0.73
1:B:706:LEU:HD13	1:B:715:LEU:HD22	1.69	0.73
1:A:487:LEU:HD21	1:A:515:GLN:HA	1.69	0.73
1:A:407:GLN:HB3	1:A:440:LYS:HD2	1.69	0.72
1:B:624:CYS:HA	1:B:629:LEU:H	1.53	0.72
1:B:309:THR:OG1	1:B:338:LYS:HG3	1.89	0.72
1:B:561:LEU:HD12	1:B:565:GLN:NE2	2.05	0.72
1:B:585:LEU:C	1:B:587:PRO:HD2	2.10	0.72
1:B:535:ILE:HD11	1:B:567:VAL:HG22	1.70	0.71
1:B:418:VAL:O	1:B:422:ALA:HB3	1.91	0.71
1:B:263:ILE:HD11	1:B:295:VAL:HG22	1.71	0.71
1:B:678:ARG:O	1:B:682:GLU:HG3	1.90	0.70
1:B:453:LEU:HD21	1:B:481:GLN:HB2	1.74	0.70
1:A:411:THR:OG1	1:A:440:LYS:HG3	1.91	0.70
1:B:714:ALA:O	1:B:715:LEU:C	2.30	0.70
1:A:282:LEU:CD2	1:A:311:GLN:HG3	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.73	0.70
1:B:457:HIS:HE1	1:B:481:GLN:HG3	1.57	0.70
1:B:586:LEU:N	1:B:587:PRO:CD	2.54	0.70
1:B:552:LEU:O	1:B:556:CYS:HB2	1.92	0.69
1:B:297:ILE:HD11	1:B:329:VAL:HG22	1.75	0.69
1:A:654:LEU:HB3	1:A:655:PRO:HD3	1.73	0.69
1:B:699:THR:HG23	1:B:702:HIS:HB2	1.75	0.69
1:B:633:GLN:HG2	1:B:669:VAL:HG11	1.75	0.69
1:B:552:LEU:N	1:B:553:PRO:CD	2.56	0.69
1:B:553:PRO:C	1:B:557:GLN:HG3	2.11	0.69
1:A:649:THR:OG1	1:A:678:ARG:HD3	1.93	0.68
1:A:604:ALA:HB2	1:A:613:LEU:HD11	1.75	0.68
1:B:670:ALA:HA	1:B:673:SER:HB2	1.75	0.68
1:B:265:LYS:CE	1:B:266:ARG:HH21	2.03	0.68
1:B:698:LEU:HD21	1:B:702:HIS:CE1	2.29	0.68
1:A:562:THR:HG23	1:A:565:GLN:OE1	1.95	0.67
1:B:615:THR:HG21	1:B:644:LYS:HG3	1.75	0.67
1:B:676:GLY:O	1:B:679:PRO:HG2	1.95	0.67
2:G:6:DC:OP2	4:G:103:HOH:O	2.13	0.66
1:A:253:LEU:HD11	1:A:279:ARG:HB3	1.78	0.66
3:H:5:DA:H2"	3:H:6:DT:H5'	1.76	0.66
1:B:372:LYS:O	1:B:376:GLU:HG3	1.96	0.65
1:B:703:LEU:N	1:B:703:LEU:HD23	2.11	0.65
1:B:237:ALA:O	1:B:241:LEU:HB2	1.96	0.65
2:G:14:DC:H2"	2:G:15:DT:C5'	2.24	0.65
3:H:12:DG:H5'	3:H:12:DG:C8	2.31	0.65
1:B:525:HIS:CD2	1:B:552:LEU:HD23	2.32	0.65
1:A:426:THR:OG1	1:A:428:GLN:HB3	1.98	0.64
1:B:681:LEU:O	1:B:683:SER:N	2.30	0.64
1:B:351:LEU:HD11	1:B:379:GLN:HB2	1.80	0.64
1:A:687:GLN:NE2	1:A:695:LEU:HD22	2.13	0.64
1:A:484:LEU:O	1:A:484:LEU:HD12	1.98	0.63
1:B:493:LEU:HD23	1:B:497:GLN:OE1	1.98	0.63
1:B:382:LEU:CD2	1:B:396:VAL:HG11	2.28	0.63
1:A:427:PRO:O	1:A:429:GLN:N	2.31	0.63
1:A:521:LEU:O	1:A:525:HIS:HB2	1.99	0.63
1:B:531:GLN:O	1:B:535:ILE:HG13	1.98	0.62
1:B:595:LEU:HD13	1:B:599:GLN:HE21	1.63	0.62
1:A:518:LEU:N	1:A:519:PRO:CD	2.62	0.62
1:B:511:LEU:O	1:B:514:VAL:N	2.32	0.62
1:B:703:LEU:HD23	1:B:703:LEU:H	1.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PRO:O	1:A:430:VAL:N	2.32	0.62
1:B:499:VAL:HG12	1:B:500:ALA:N	2.14	0.62
1:B:265:LYS:HE3	1:B:266:ARG:HH21	1.63	0.61
3:H:9:DA:H2'	3:H:10:DG:C8	2.36	0.61
1:B:524:ALA:O	1:B:525:HIS:C	2.39	0.61
1:A:239:GLU:O	1:A:243:THR:OG1	2.16	0.61
1:A:655:PRO:O	1:A:659:GLN:CG	2.46	0.61
1:B:570:ALA:HB2	1:B:579:LEU:HD11	1.83	0.61
1:A:491:HIS:CD2	1:A:518:LEU:HD23	2.36	0.60
1:B:494:THR:O	1:B:498:VAL:HG23	2.00	0.60
2:G:14:DC:C2'	2:G:15:DT:H5"	2.26	0.60
1:B:547:THR:HG22	1:B:579:LEU:HD12	1.83	0.60
1:B:714:ALA:O	1:B:717:ALA:CA	2.49	0.60
1:B:324:THR:HG23	1:B:327:GLN:OE1	2.02	0.60
1:B:335:ASP:HB2	1:B:369:ASP:OD2	2.01	0.60
1:A:382:LEU:HG	1:A:396:VAL:HG11	1.84	0.60
1:A:656:VAL:O	1:A:660:ALA:HB3	2.01	0.60
1:A:450:LEU:N	1:A:451:PRO:HD2	2.15	0.60
1:A:292:GLU:CD	1:A:292:GLU:N	2.55	0.60
1:A:684:ILE:HG12	1:A:715:LEU:HD21	1.82	0.60
1:B:715:LEU:H	1:B:715:LEU:CD2	2.13	0.60
1:B:550:ARG:HB3	1:B:551:LEU:HD23	1.83	0.60
1:B:595:LEU:HD11	1:B:635:VAL:HG22	1.84	0.60
1:B:450:LEU:O	1:B:454:CYS:HB2	2.01	0.59
1:B:572:HIS:NE2	1:B:605:SER:O	2.35	0.59
1:A:486:VAL:O	1:A:488:CYS:N	2.34	0.59
1:B:714:ALA:O	1:B:717:ALA:HB3	2.02	0.59
1:A:620:LEU:HG	1:A:634:VAL:HG11	1.83	0.59
1:B:553:PRO:O	1:B:557:GLN:CB	2.50	0.59
1:B:620:LEU:N	1:B:621:PRO:HD2	2.18	0.59
1:A:287:LEU:CD1	1:A:311:GLN:HA	2.30	0.59
1:A:519:PRO:O	1:A:520:VAL:C	2.41	0.59
1:A:519:PRO:O	1:A:521:LEU:N	2.36	0.59
3:H:5:DA:H2"	3:H:6:DT:C5'	2.32	0.59
1:B:475:GLN:O	1:B:479:THR:OG1	2.19	0.59
1:A:368:HIS:NE2	1:A:401:SER:O	2.35	0.59
1:A:416:LEU:N	1:A:417:PRO:HD2	2.18	0.59
1:B:525:HIS:HD2	1:B:552:LEU:HD23	1.68	0.59
1:B:260:LEU:HD13	1:B:260:LEU:H	1.68	0.58
1:B:657:LEU:HD22	1:B:663:LEU:HD13	1.84	0.58
3:H:12:DG:H5'	3:H:12:DG:H8	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LEU:C	1:B:455:GLN:H	2.06	0.58
1:B:493:LEU:HD23	1:B:497:GLN:CD	2.24	0.58
1:B:586:LEU:N	1:B:587:PRO:HD2	2.17	0.58
1:B:597:PRO:O	1:B:600:VAL:N	2.35	0.58
1:B:449:LEU:HA	1:B:452:VAL:HG13	1.84	0.58
1:B:688:LEU:HD21	1:B:700:ASN:ND2	2.18	0.58
1:A:473:GLY:O	1:A:474:LYS:C	2.41	0.58
1:A:473:GLY:O	1:A:476:ALA:N	2.37	0.58
1:A:497:GLN:HG2	1:A:533:VAL:HG11	1.85	0.58
1:B:348:LEU:O	1:B:352:CYS:SG	2.62	0.58
1:B:655:PRO:O	1:B:659:GLN:HB2	2.04	0.58
1:B:571:SER:C	1:B:572:HIS:HD1	2.07	0.57
1:B:373:GLN:HG3	1:B:406:LYS:HD2	1.86	0.57
1:A:253:LEU:HB3	1:A:255:LEU:HD21	1.86	0.57
1:A:399:ILE:HD11	1:A:431:VAL:HG13	1.87	0.57
1:B:649:THR:HG23	1:B:652:ARG:NH2	2.19	0.57
2:G:4:DC:H42	3:H:12:DG:H1	1.51	0.57
1:A:445:THR:OG1	1:A:474:LYS:CG	2.52	0.57
1:B:343:THR:OG1	1:B:372:LYS:HG3	2.06	0.56
1:B:606:ASN:HB3	1:B:641:ASP:OD2	2.06	0.56
1:A:467:ILE:HD11	1:A:499:VAL:HG23	1.87	0.56
1:A:718:VAL:O	1:A:720:LYS:N	2.39	0.56
1:B:271:ALA:O	1:B:275:VAL:HG23	2.06	0.56
1:B:480:VAL:O	1:B:484:LEU:HB2	2.05	0.56
1:B:450:LEU:HD12	1:B:454:CYS:SG	2.46	0.56
3:H:5:DA:H2'	3:H:6:DT:H71	1.88	0.56
1:B:327:GLN:NE2	1:B:363:VAL:HG21	2.21	0.56
1:B:604:ALA:HB2	1:B:613:LEU:HD21	1.88	0.56
1:B:255:LEU:HD21	1:B:295:VAL:CG2	2.36	0.55
1:B:582:VAL:HG23	1:B:613:LEU:HD11	1.87	0.55
1:B:509:GLN:HB3	1:B:542:LYS:HD2	1.89	0.55
1:A:475:GLN:HB3	1:A:508:LYS:HD3	1.89	0.55
2:I:11:DT:H2"	2:I:12:DC:O5'	2.07	0.55
1:B:561:LEU:HD12	1:B:565:GLN:HE22	1.72	0.55
1:B:702:HIS:O	1:B:704:VAL:N	2.40	0.55
1:B:712:ARG:N	1:B:713:PRO:CD	2.69	0.55
1:A:487:LEU:HD21	1:A:515:GLN:CA	2.36	0.55
1:B:255:LEU:HA	1:B:259:GLN:OE1	2.06	0.55
1:B:460:THR:OG1	1:B:462:GLN:OE1	2.25	0.55
1:B:494:THR:OG1	1:B:497:GLN:HG2	2.06	0.54
1:B:623:LEU:O	1:B:628:GLY:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:THR:O	1:A:551:LEU:HB2	2.07	0.54
1:B:589:LEU:HD12	1:B:600:VAL:HG22	1.89	0.54
1:B:562:THR:O	1:B:566:VAL:HG23	2.06	0.54
1:A:416:LEU:HD12	1:A:430:VAL:HG11	1.90	0.54
1:A:445:THR:HG22	1:A:477:LEU:HD13	1.90	0.54
1:B:343:THR:CG2	1:B:375:LEU:HD12	2.38	0.54
1:B:701:ASP:O	1:B:704:VAL:HB	2.08	0.54
1:B:714:ALA:O	1:B:717:ALA:CB	2.56	0.54
1:A:463:GLN:O	1:A:466:ALA:HB3	2.07	0.54
1:B:351:LEU:O	1:B:357:LEU:CB	2.45	0.54
1:A:253:LEU:CD1	1:A:279:ARG:HB3	2.37	0.54
1:B:392:THR:OG1	1:B:395:GLN:HG3	2.07	0.54
1:A:689:SER:C	1:A:691:PRO:HD3	2.28	0.54
1:A:718:VAL:C	1:A:720:LYS:N	2.61	0.54
1:B:334:HIS:HB3	1:B:369:ASP:OD1	2.08	0.53
1:B:524:ALA:O	1:B:526:GLY:N	2.41	0.53
1:B:596:THR:O	1:B:599:GLN:HB2	2.08	0.53
1:A:638:ALA:HB2	1:A:647:LEU:HD11	1.90	0.53
1:B:460:THR:O	1:B:464:VAL:HG23	2.08	0.53
1:B:617:GLN:O	1:B:619:LEU:N	2.39	0.53
1:A:519:PRO:O	1:A:522:CYS:N	2.41	0.53
1:A:578:ALA:O	1:A:582:VAL:HG23	2.08	0.53
2:I:12:DC:H2"	2:I:13:DT:O5'	2.08	0.53
1:B:425:LEU:O	1:B:426:THR:C	2.46	0.53
1:B:487:LEU:HD13	1:B:493:LEU:HD13	1.91	0.53
1:A:547:THR:OG1	1:A:576:LYS:HG3	2.09	0.53
1:B:585:LEU:HD21	1:B:617:GLN:OE1	2.07	0.53
1:A:412:VAL:HG13	1:A:416:LEU:HD13	1.90	0.53
1:B:645:GLN:HB3	1:B:678:ARG:HD2	1.90	0.53
1:A:445:THR:OG1	1:A:474:LYS:HG3	2.08	0.53
1:B:255:LEU:CD2	1:B:295:VAL:CG2	2.87	0.52
1:B:615:THR:OG1	1:B:647:LEU:HD12	2.10	0.52
1:A:581:THR:OG1	1:A:610:LYS:HB2	2.09	0.52
3:H:0:DG:H2"	3:H:1:DA:C8	2.44	0.52
1:A:297:ILE:CG2	1:A:307:LEU:HD13	2.38	0.52
1:A:348:LEU:HB3	1:A:349:PRO:HD3	1.91	0.52
1:B:681:LEU:O	1:B:682:GLU:C	2.46	0.52
1:B:255:LEU:HD21	1:B:295:VAL:HG23	1.91	0.52
1:B:453:LEU:HD21	1:B:481:GLN:CB	2.38	0.52
1:A:496:GLN:O	1:A:499:VAL:HG12	2.09	0.52
1:B:255:LEU:HB3	1:B:260:LEU:CD1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ALA:O	1:B:402:ASN:N	2.41	0.52
1:B:446:VAL:O	1:B:450:LEU:HB3	2.08	0.52
1:B:566:VAL:HA	1:B:569:ILE:HD12	1.91	0.52
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.91	0.52
1:A:402:ASN:OD1	4:A:805:HOH:O	2.19	0.52
1:B:493:LEU:CG	1:B:497:GLN:OE1	2.58	0.52
1:B:562:THR:N	1:B:565:GLN:OE1	2.38	0.52
2:I:12:DC:OP2	4:I:106:HOH:O	2.19	0.52
1:B:411:THR:OG1	1:B:440:LYS:HG3	2.10	0.52
1:B:457:HIS:CE1	1:B:481:GLN:HG3	2.43	0.52
1:B:712:ARG:N	1:B:713:PRO:HD2	2.25	0.52
1:B:453:LEU:HD23	1:B:457:HIS:ND1	2.25	0.51
1:A:429:GLN:O	1:A:433:ILE:HG13	2.11	0.51
1:B:232:TRP:CD1	1:B:233:SER:N	2.78	0.51
1:B:476:ALA:O	1:B:480:VAL:HG23	2.11	0.51
1:A:467:ILE:HD11	1:A:499:VAL:CG2	2.41	0.51
1:B:405:GLY:O	1:B:406:LYS:C	2.49	0.51
1:A:666:GLN:CD	1:A:666:GLN:H	2.14	0.51
1:A:687:GLN:CD	1:A:695:LEU:HD22	2.31	0.51
1:A:552:LEU:N	1:A:553:PRO:HD2	2.26	0.51
1:B:479:THR:OG1	1:B:508:LYS:HG3	2.11	0.51
1:B:659:GLN:O	1:B:660:ALA:HB2	2.11	0.51
2:G:14:DC:H2'	2:G:15:DT:H72	1.93	0.51
1:A:488:CYS:HA	1:A:493:LEU:O	2.11	0.51
1:A:718:VAL:C	1:A:720:LYS:H	2.14	0.51
1:A:343:THR:HG23	1:A:347:LEU:HD12	1.92	0.51
2:I:14:DC:C6	2:I:15:DT:H72	2.46	0.51
1:B:260:LEU:CD1	1:B:260:LEU:N	2.74	0.51
1:B:550:ARG:NH2	1:B:551:LEU:HD21	2.26	0.51
1:A:623:LEU:HD23	1:A:634:VAL:HG22	1.93	0.50
1:B:571:SER:O	1:B:572:HIS:ND1	2.28	0.50
1:B:671:ILE:HG22	1:B:672:ALA:N	2.26	0.50
1:B:663:LEU:HG	1:B:667:GLN:OE1	2.10	0.50
1:A:487:LEU:HD23	1:A:491:HIS:ND1	2.26	0.50
1:B:641:ASP:OD2	1:B:641:ASP:N	2.45	0.50
1:A:343:THR:OG1	1:A:372:LYS:HB2	2.11	0.50
1:A:623:LEU:O	1:A:624:CYS:C	2.49	0.50
1:A:634:VAL:HA	1:A:637:ILE:HD12	1.94	0.50
1:B:703:LEU:H	1:B:703:LEU:CD2	2.19	0.50
1:B:314:LEU:HG	1:B:328:VAL:HG21	1.93	0.50
1:B:348:LEU:CD1	1:B:352:CYS:SG	2.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:CG	2:I:5:DC:H5"	2.41	0.50
1:B:617:GLN:C	1:B:619:LEU:H	2.15	0.50
1:B:678:ARG:N	1:B:679:PRO:HD2	2.26	0.50
1:A:339:GLN:HB3	1:A:372:LYS:HD3	1.94	0.50
1:B:260:LEU:HD13	1:B:260:LEU:N	2.27	0.49
1:B:640:HIS:CD2	1:B:674:ASN:HA	2.46	0.49
1:B:440:LYS:O	1:B:444:GLU:HG3	2.11	0.49
3:H:10:DG:H1'	3:H:11:DG:H5'	1.94	0.49
1:B:585:LEU:O	1:B:589:LEU:HB2	2.13	0.49
1:B:350:VAL:O	1:B:354:ALA:N	2.45	0.49
1:B:714:ALA:HA	1:B:717:ALA:HB3	1.94	0.49
1:A:491:HIS:CB	1:A:518:LEU:HD23	2.40	0.49
1:B:355:HIS:CE1	1:B:383:PRO:HD3	2.48	0.49
1:A:406:LYS:O	1:A:410:GLU:HG3	2.12	0.49
1:A:525:HIS:HE1	1:A:549:GLN:HA	1.78	0.49
3:J:10:DG:H2"	3:J:11:DG:H5'	1.94	0.49
1:B:556:CYS:O	1:B:557:GLN:HG2	2.12	0.49
1:A:486:VAL:O	1:A:487:LEU:C	2.50	0.49
1:A:698:LEU:HD22	1:A:702:HIS:CD2	2.48	0.49
1:B:395:GLN:O	1:B:398:ALA:HB3	2.13	0.49
1:B:711:GLY:C	1:B:713:PRO:CD	2.78	0.49
1:A:305:GLN:OE1	1:A:305:GLN:HA	2.13	0.48
1:B:370:GLY:O	1:B:373:GLN:N	2.45	0.48
1:B:420:CYS:O	1:B:421:GLN:O	2.30	0.48
1:B:613:LEU:O	1:B:614:GLU:C	2.52	0.48
1:A:314:LEU:N	1:A:315:PRO:HD2	2.28	0.48
1:A:528:THR:HG23	1:A:531:GLN:OE1	2.14	0.48
1:B:417:PRO:O	1:B:421:GLN:HG2	2.13	0.48
3:H:9:DA:H2'	3:H:10:DG:H8	1.77	0.48
1:A:445:THR:OG1	1:A:474:LYS:HG2	2.12	0.48
1:A:552:LEU:HD12	1:A:552:LEU:O	2.12	0.48
1:A:590:CYS:SG	1:A:595:LEU:O	2.71	0.48
1:A:321:HIS:HB3	1:A:348:LEU:CD2	2.44	0.48
1:A:684:ILE:HG12	1:A:715:LEU:CD2	2.42	0.48
1:B:359:PRO:HD2	1:B:360:GLU:OE2	2.13	0.48
1:A:468:ALA:C	1:A:470:ASN:H	2.17	0.48
1:B:244:VAL:O	1:B:245:ALA:C	2.51	0.48
1:B:713:PRO:O	1:B:714:ALA:C	2.51	0.48
3:J:10:DG:C2'	3:J:11:DG:H5'	2.44	0.48
1:B:383:PRO:O	1:B:387:GLN:HG3	2.14	0.48
1:B:720:LYS:HE2	1:B:720:LYS:HB2	1.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:ARG:HB3	1:B:584:ARG:CZ	2.44	0.47
1:A:392:THR:OG1	1:A:395:GLN:HG3	2.14	0.47
1:B:417:PRO:O	1:B:421:GLN:CG	2.62	0.47
1:B:450:LEU:N	1:B:451:PRO:HD2	2.29	0.47
1:B:715:LEU:CD2	1:B:715:LEU:N	2.72	0.47
1:B:513:THR:OG1	1:B:542:LYS:HG3	2.15	0.47
1:A:382:LEU:HB3	1:A:383:PRO:HD3	1.95	0.47
1:A:631:PRO:O	1:A:635:VAL:HG23	2.14	0.47
2:I:12:DC:H2'	2:I:13:DT:H71	1.96	0.47
1:B:624:CYS:SG	1:B:629:LEU:O	2.71	0.47
1:B:712:ARG:HH21	2:G:15:DT:P	2.36	0.47
1:A:276:HIS:O	1:A:279:ARG:HG2	2.14	0.47
1:A:314:LEU:HD12	1:A:328:VAL:HG11	1.96	0.47
1:B:351:LEU:HD11	1:B:379:GLN:CB	2.43	0.47
3:H:14:DC:H2"	3:H:15:DA:C8	2.49	0.47
3:J:13:DA:H2"	3:J:14:DC:O5'	2.14	0.47
1:B:668:VAL:O	1:B:671:ILE:HB	2.14	0.47
1:B:536:ALA:HB2	1:B:545:LEU:HD11	1.95	0.47
1:B:271:ALA:O	1:B:274:ALA:HB3	2.14	0.47
1:A:657:LEU:HD21	1:A:685:VAL:HG22	1.97	0.47
1:B:343:THR:HG22	1:B:375:LEU:HD12	1.95	0.47
1:A:325:PRO:O	1:A:329:VAL:HG23	2.15	0.46
1:B:529:PRO:O	1:B:533:VAL:HB	2.15	0.46
1:A:322:GLY:O	1:A:323:LEU:HD23	2.16	0.46
1:B:324:THR:OG1	1:B:327:GLN:HG3	2.15	0.46
1:A:518:LEU:N	1:A:519:PRO:HD2	2.29	0.46
1:B:426:THR:O	1:B:427:PRO:C	2.53	0.46
1:B:552:LEU:N	1:B:553:PRO:HD2	2.31	0.46
1:A:463:GLN:O	1:A:467:ILE:HG13	2.16	0.46
1:A:302:GLY:O	1:A:305:GLN:N	2.49	0.46
1:B:249:ARG:HH21	1:B:257:THR:HG23	1.61	0.46
1:B:400:ALA:C	1:B:402:ASN:H	2.17	0.46
1:A:289:LEU:HD23	1:A:289:LEU:N	2.30	0.46
1:A:381:LEU:HD12	1:A:409:LEU:HB3	1.96	0.46
1:A:484:LEU:N	1:A:485:PRO:HD2	2.30	0.46
1:A:302:GLY:O	1:A:304:LYS:N	2.48	0.46
1:A:313:LEU:O	1:A:314:LEU:C	2.54	0.46
1:A:427:PRO:O	1:A:428:GLN:C	2.54	0.46
1:A:519:PRO:HB2	1:A:520:VAL:H	1.60	0.46
1:B:664:THR:O	1:B:667:GLN:HB2	2.16	0.46
1:A:716:ASP:O	1:A:719:LYS:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:O	1:A:354:ALA:HB3	2.16	0.46
1:A:484:LEU:HD12	1:A:484:LEU:C	2.35	0.46
1:A:531:GLN:O	1:A:534:ALA:HB3	2.16	0.46
1:B:419:LEU:HD21	1:B:447:GLN:HB2	1.98	0.46
1:B:704:VAL:O	1:B:705:ALA:C	2.54	0.46
1:B:706:LEU:O	1:B:708:CYS:N	2.48	0.46
1:B:511:LEU:O	1:B:512:GLU:C	2.54	0.45
1:B:625:GLN:OE1	1:B:626:ALA:HB2	2.15	0.45
1:A:468:ALA:O	1:A:470:ASN:N	2.41	0.45
1:A:525:HIS:CE1	1:A:549:GLN:HA	2.51	0.45
1:B:236:ARG:O	1:B:237:ALA:C	2.54	0.45
1:B:425:LEU:CD1	1:B:429:GLN:OE1	2.52	0.45
1:B:550:ARG:CZ	1:B:551:LEU:HD21	2.47	0.45
3:H:10:DG:H2"	3:H:11:DG:OP2	2.16	0.45
1:B:393:PRO:O	1:B:395:GLN:N	2.49	0.45
1:B:642:GLY:O	1:B:643:GLY:C	2.54	0.45
1:A:382:LEU:HD23	1:A:386:CYS:SG	2.57	0.45
1:A:596:THR:O	1:A:600:VAL:HG23	2.16	0.45
1:B:382:LEU:HD23	1:B:382:LEU:HA	1.73	0.45
1:A:395:GLN:OE1	1:A:431:VAL:HG21	2.17	0.45
2:I:10:DA:H2"	2:I:11:DT:O5'	2.17	0.45
1:B:555:LEU:HA	1:B:559:HIS:HB2	1.99	0.45
1:B:664:THR:OG1	1:B:667:GLN:N	2.46	0.45
1:A:278:TRP:CB	1:A:311:GLN:HE22	2.30	0.45
1:A:487:LEU:HD21	1:A:515:GLN:CB	2.46	0.45
1:A:616:VAL:HG13	1:A:620:LEU:HD12	1.99	0.45
1:B:303:GLY:O	1:B:307:LEU:HG	2.17	0.45
1:A:256:ASP:OD2	1:A:259:GLN:HG3	2.17	0.44
1:A:550:ARG:HD2	1:A:551:LEU:HD23	1.99	0.44
1:A:343:THR:CB	1:A:372:LYS:HB2	2.46	0.44
1:A:420:CYS:HA	1:A:425:LEU:O	2.18	0.44
1:A:569:ILE:HD13	1:A:582:VAL:HG21	1.99	0.44
1:B:426:THR:O	1:B:428:GLN:N	2.50	0.44
1:A:486:VAL:C	1:A:488:CYS:N	2.70	0.44
1:A:597:PRO:O	1:A:601:VAL:HG23	2.18	0.44
1:B:493:LEU:CD2	1:B:497:GLN:OE1	2.63	0.44
1:B:654:LEU:N	1:B:655:PRO:HD2	2.33	0.44
1:B:405:GLY:O	1:B:408:ALA:N	2.51	0.44
1:B:453:LEU:C	1:B:455:GLN:N	2.70	0.44
1:A:324:THR:OG1	1:A:327:GLN:HG3	2.18	0.44
1:A:688:LEU:O	1:A:691:PRO:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.99	0.44
1:B:255:LEU:HD22	1:B:259:GLN:HB3	2.00	0.44
1:B:255:LEU:HB2	1:B:260:LEU:HD11	2.00	0.44
1:B:352:CYS:HA	1:B:357:LEU:H	1.83	0.44
1:B:393:PRO:O	1:B:396:VAL:N	2.51	0.44
1:A:367:SER:O	1:A:368:HIS:ND1	2.51	0.44
1:A:444:GLU:H	1:A:444:GLU:HG2	1.68	0.44
1:A:659:GLN:HG2	1:A:659:GLN:H	1.42	0.44
1:B:715:LEU:O	1:B:716:ASP:C	2.56	0.44
1:B:255:LEU:CB	1:B:260:LEU:HD11	2.48	0.43
1:A:302:GLY:O	1:A:303:GLY:C	2.56	0.43
1:A:591:GLN:C	1:A:593:HIS:H	2.20	0.43
1:B:622:VAL:HA	1:B:625:GLN:HB3	1.99	0.43
1:A:598:GLU:CD	1:A:598:GLU:H	2.21	0.43
1:B:331:ILE:HG21	1:B:341:LEU:HD23	1.99	0.43
1:A:620:LEU:HD23	1:A:620:LEU:O	2.18	0.43
1:B:421:GLN:HB2	1:B:422:ALA:H	1.61	0.43
1:B:658:CYS:SG	1:B:665:PRO:HA	2.58	0.43
1:A:468:ALA:CB	1:A:477:LEU:HD11	2.45	0.43
1:A:585:LEU:HD23	1:A:585:LEU:HA	1.81	0.43
1:B:552:LEU:HB3	1:B:553:PRO:HD3	2.00	0.43
1:B:663:LEU:HD23	1:B:664:THR:O	2.18	0.43
1:A:538:ASN:OD1	1:A:571:SER:O	2.36	0.43
1:B:236:ARG:O	1:B:239:GLU:N	2.51	0.43
1:B:460:THR:HG23	1:B:463:GLN:CD	2.39	0.43
1:B:595:LEU:CD1	1:B:599:GLN:HE21	2.28	0.43
1:B:616:VAL:O	1:B:620:LEU:HB2	2.18	0.43
1:B:702:HIS:O	1:B:703:LEU:C	2.57	0.43
1:B:706:LEU:O	1:B:709:LEU:N	2.52	0.43
3:H:5:DA:H2'	3:H:6:DT:C6	2.54	0.43
1:A:356:GLY:O	1:A:357:LEU:HD23	2.17	0.43
1:B:475:GLN:HB3	1:B:508:LYS:HD2	2.00	0.43
1:B:505:ILE:HG21	2:G:10:DA:N7	2.34	0.43
1:A:457:HIS:HB2	1:A:459:LEU:HD22	2.00	0.43
1:A:487:LEU:O	1:A:491:HIS:HB2	2.18	0.43
1:B:255:LEU:CD2	1:B:295:VAL:HG21	2.48	0.43
1:A:249:ARG:NH1	1:A:257:THR:OG1	2.47	0.43
1:A:670:ALA:HB1	1:A:708:CYS:SG	2.59	0.43
1:B:317:LEU:O	1:B:321:HIS:HB2	2.19	0.43
1:B:335:ASP:HB2	1:B:369:ASP:CG	2.39	0.43
1:B:482:ARG:HE	1:B:482:ARG:HB3	1.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:THR:O	1:B:585:LEU:HB2	2.19	0.42
1:B:653:LEU:HD13	1:B:685:VAL:HG21	2.00	0.42
1:A:314:LEU:HD12	1:A:328:VAL:CG1	2.49	0.42
1:A:252:PRO:HD2	1:A:279:ARG:HB2	2.01	0.42
1:A:278:TRP:HB3	1:A:311:GLN:NE2	2.35	0.42
1:A:522:CYS:HA	1:A:527:LEU:O	2.19	0.42
1:B:659:GLN:O	1:B:660:ALA:CB	2.67	0.42
1:A:509:GLN:HB3	1:A:542:LYS:HD3	2.02	0.42
1:A:627:HIS:ND1	1:A:654:LEU:HD22	2.34	0.42
1:B:329:VAL:O	1:B:333:SER:N	2.51	0.42
1:B:350:VAL:HG22	1:B:351:LEU:HD13	2.01	0.42
1:B:450:LEU:N	1:B:451:PRO:CD	2.82	0.42
1:A:577:GLN:HB3	1:A:610:LYS:HD2	2.00	0.42
1:B:253:LEU:HD12	1:B:291:PRO:HA	2.00	0.42
1:B:357:LEU:HD22	1:B:361:GLN:HB2	2.01	0.42
1:B:586:LEU:HD13	1:B:600:VAL:HG11	2.01	0.42
1:B:329:VAL:O	1:B:332:ALA:N	2.53	0.42
1:B:393:PRO:O	1:B:394:GLU:C	2.57	0.42
1:B:419:LEU:HD21	1:B:447:GLN:HG3	2.00	0.42
1:B:548:VAL:O	1:B:552:LEU:HB2	2.20	0.42
1:A:377:THR:OG1	1:A:406:LYS:HG3	2.18	0.42
1:A:629:LEU:HD23	1:A:629:LEU:HA	1.89	0.42
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.83	0.42
1:B:348:LEU:HD13	1:B:352:CYS:HG	1.82	0.42
1:B:425:LEU:HD12	1:B:425:LEU:HA	1.90	0.42
1:B:596:THR:O	1:B:600:VAL:HG23	2.19	0.42
1:B:677:GLY:O	1:B:678:ARG:C	2.58	0.42
1:A:448:ARG:HG2	1:A:449:LEU:HD23	2.02	0.42
1:A:657:LEU:HD23	1:A:657:LEU:HA	1.87	0.42
1:A:699:THR:HG23	1:A:702:HIS:CD2	2.54	0.42
2:I:3:DT:C2	2:I:4:DC:C6	3.07	0.42
1:B:370:GLY:O	1:B:371:GLY:C	2.57	0.42
1:B:487:LEU:HD12	1:B:498:VAL:HG22	2.00	0.42
1:A:510:ALA:O	1:A:514:VAL:HG23	2.20	0.42
1:A:684:ILE:CG1	1:A:715:LEU:HD21	2.50	0.42
1:B:630:THR:OG1	1:B:632:GLU:N	2.53	0.42
1:A:446:VAL:O	1:A:447:GLN:C	2.58	0.42
1:A:457:HIS:CD2	1:A:457:HIS:N	2.87	0.42
1:A:619:LEU:HD12	1:A:619:LEU:HA	1.82	0.42
1:B:484:LEU:N	1:B:485:PRO:CD	2.83	0.42
1:B:522:CYS:SG	1:B:527:LEU:O	2.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:DT:H3	3:H:15:DA:H2	1.65	0.42
1:A:598:GLU:CD	1:A:598:GLU:N	2.73	0.41
1:A:698:LEU:HD22	1:A:702:HIS:CB	2.50	0.41
1:B:364:ALA:O	1:B:368:HIS:NE2	2.53	0.41
1:B:609:GLY:O	1:B:610:LYS:C	2.57	0.41
1:A:475:GLN:HB2	4:I:104:HOH:O	2.20	0.41
1:A:659:GLN:O	1:A:661:HIS:N	2.53	0.41
1:B:293:GLN:O	1:B:297:ILE:HG13	2.20	0.41
1:B:702:HIS:C	1:B:704:VAL:N	2.74	0.41
1:A:582:VAL:O	1:A:585:LEU:N	2.50	0.41
1:A:684:ILE:CD1	1:A:715:LEU:HD21	2.51	0.41
1:A:407:GLN:CG	2:I:6:DC:H5"	2.50	0.41
1:B:511:LEU:O	1:B:514:VAL:HG12	2.19	0.41
1:B:555:LEU:H	1:B:555:LEU:HG	1.70	0.41
1:B:687:GLN:O	1:B:691:PRO:HB3	2.20	0.41
1:A:287:LEU:O	1:A:289:LEU:HD23	2.21	0.41
1:B:669:VAL:O	1:B:673:SER:N	2.54	0.41
1:B:290:THR:N	1:B:293:GLN:OE1	2.53	0.41
1:B:350:VAL:O	1:B:354:ALA:CA	2.69	0.41
1:B:575:GLY:O	1:B:578:ALA:HB3	2.21	0.41
1:A:582:VAL:O	1:A:583:GLN:C	2.59	0.41
1:A:659:GLN:HB2	1:A:660:ALA:H	1.58	0.41
1:B:256:ASP:HB2	1:B:257:THR:H	1.75	0.41
1:A:282:LEU:CG	1:A:311:GLN:HE21	2.34	0.41
1:A:590:CYS:HA	1:A:595:LEU:O	2.21	0.41
1:B:244:VAL:HG12	1:B:245:ALA:N	2.35	0.41
1:B:320:ALA:O	1:B:321:HIS:ND1	2.53	0.41
1:B:416:LEU:CD2	1:B:420:CYS:SG	3.09	0.41
1:B:687:GLN:O	1:B:687:GLN:NE2	2.26	0.41
1:B:236:ARG:O	1:B:238:LEU:N	2.54	0.41
1:B:704:VAL:HG12	1:B:705:ALA:N	2.34	0.41
1:A:300:HIS:HB3	1:A:335:ASP:OD1	2.22	0.40
1:A:361:GLN:O	1:A:364:ALA:HB3	2.20	0.40
1:B:348:LEU:HD13	1:B:348:LEU:O	2.22	0.40
1:B:585:LEU:C	1:B:587:PRO:CD	2.81	0.40
1:B:629:LEU:HB3	1:B:633:GLN:OE1	2.20	0.40
1:A:471:GLY:O	1:A:472:GLY:C	2.58	0.40
1:A:659:GLN:HE21	1:A:659:GLN:HB3	1.65	0.40
1:B:434:ALA:HB2	1:B:443:LEU:HD11	2.03	0.40
2:I:16:DC:H6	2:I:16:DC:H2'	1.69	0.40
1:B:678:ARG:HB3	1:B:679:PRO:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TRP:HB3	1:A:311:GLN:HE22	1.85	0.40
1:A:454:CYS:SG	1:A:461:PRO:N	2.95	0.40
1:B:365:ILE:HD11	1:B:397:VAL:HG13	2.02	0.40
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.77	0.40
1:B:314:LEU:N	1:B:315:PRO:CD	2.84	0.40
1:B:326:GLN:O	1:B:327:GLN:C	2.59	0.40
1:B:361:GLN:O	1:B:365:ILE:HG13	2.22	0.40
1:B:387:GLN:HG3	1:B:387:GLN:H	1.60	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLN:OE1	1:B:448:ARG:O[2_444]	1.65	0.55

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	484/499 (97%)	399 (82%)	62 (13%)	23 (5%)	2	4
1	B	482/499 (97%)	348 (72%)	87 (18%)	47 (10%)	0	0
All	All	966/998 (97%)	747 (77%)	149 (15%)	70 (7%)	1	1

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	GLY
1	A	428	GLN
1	A	486	VAL
1	A	519	PRO
1	A	520	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	625	GLN
1	A	659	GLN
1	A	660	ALA
1	B	421	GLN
1	B	511	LEU
1	B	589	LEU
1	B	621	PRO
1	B	660	ALA
1	B	706	LEU
1	B	715	LEU
1	A	265	LYS
1	A	452	VAL
1	A	487	LEU
1	A	587	PRO
1	A	592	ALA
1	B	422	ALA
1	B	438	GLY
1	B	519	PRO
1	B	525	HIS
1	B	591	GLN
1	B	628	GLY
1	B	643	GLY
1	B	656	VAL
1	B	681	LEU
1	B	682	GLU
1	B	702	HIS
1	B	703	LEU
1	B	704	VAL
1	B	707	ALA
1	B	713	PRO
1	B	714	ALA
1	A	353	GLN
1	A	427	PRO
1	A	623	LEU
1	A	624	CYS
1	A	719	LYS
1	B	383	PRO
1	B	454	CYS
1	B	512	GLU
1	B	587	PRO
1	B	598	GLU
1	A	474	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	233	SER
1	B	451	PRO
1	B	618	ARG
1	A	456	ALA
1	A	627	HIS
1	B	394	GLU
1	B	401	SER
1	B	485	PRO
1	B	592	ALA
1	B	597	PRO
1	B	654	LEU
1	A	383	PRO
1	A	626	ALA
1	B	288	ASN
1	B	349	PRO
1	B	622	VAL
1	B	655	PRO
1	B	371	GLY
1	B	553	PRO
1	B	356	GLY
1	B	662	GLY
1	B	427	PRO
1	B	685	VAL

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	371/383 (97%)	324 (87%)	47 (13%)	4 8
1	B	372/383 (97%)	298 (80%)	74 (20%)	1 1
All	All	743/766 (97%)	622 (84%)	121 (16%)	2 3

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	A	243	THR
1	A	254	GLN
1	A	266	ARG
1	A	270	THR
1	A	289	LEU
1	A	292	GLU
1	A	299	SER
1	A	307	LEU
1	A	308	GLU
1	A	326	GLN
1	A	350	VAL
1	A	382	LEU
1	A	384	VAL
1	A	447	GLN
1	A	453	LEU
1	A	460	THR
1	A	470	ASN
1	A	488	CYS
1	A	489	GLN
1	A	499	VAL
1	A	505	ILE
1	A	523	GLN
1	A	527	LEU
1	A	551	LEU
1	A	552	LEU
1	A	562	THR
1	A	564	GLN
1	A	581	THR
1	A	588	VAL
1	A	596	THR
1	A	619	LEU
1	A	620	LEU
1	A	623	LEU
1	A	630	THR
1	A	641	ASP
1	A	651	GLN
1	A	659	GLN
1	A	664	THR
1	A	666	GLN
1	A	678	ARG
1	A	683	SER
1	A	689	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	690	ARG
1	A	695	LEU
1	A	709	LEU
1	A	719	LYS
1	B	233	SER
1	B	241	LEU
1	B	256	ASP
1	B	257	THR
1	B	260	LEU
1	B	261	LEU
1	B	262	LYS
1	B	266	ARG
1	B	269	VAL
1	B	270	THR
1	B	283	THR
1	B	324	THR
1	B	339	GLN
1	B	345	GLN
1	B	350	VAL
1	B	353	GLN
1	B	357	LEU
1	B	358	THR
1	B	382	LEU
1	B	384	VAL
1	B	387	GLN
1	B	412	VAL
1	B	413	GLN
1	B	416	LEU
1	B	421	GLN
1	B	425	LEU
1	B	426	THR
1	B	446	VAL
1	B	450	LEU
1	B	455	GLN
1	B	460	THR
1	B	479	THR
1	B	482	ARG
1	B	484	LEU
1	B	486	VAL
1	B	487	LEU
1	B	491	HIS
1	B	497	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	504	ASN
1	B	512	GLU
1	B	514	VAL
1	B	521	LEU
1	B	528	THR
1	B	533	VAL
1	B	555	LEU
1	B	561	LEU
1	B	584	ARG
1	B	589	LEU
1	B	595	LEU
1	B	596	THR
1	B	606	ASN
1	B	618	ARG
1	B	620	LEU
1	B	629	LEU
1	B	630	THR
1	B	634	VAL
1	B	639	SER
1	B	641	ASP
1	B	657	LEU
1	B	663	LEU
1	B	664	THR
1	B	666	GLN
1	B	674	ASN
1	B	683	SER
1	B	684	ILE
1	B	687	GLN
1	B	688	LEU
1	B	690	ARG
1	B	692	ASP
1	B	699	THR
1	B	703	LEU
1	B	709	LEU
1	B	715	LEU
1	B	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	300	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	311	GLN
1	A	504	ASN
1	A	525	HIS
1	A	659	GLN
1	A	702	HIS
1	B	311	GLN
1	B	355	HIS
1	B	525	HIS
1	B	543	GLN
1	B	557	GLN
1	B	599	GLN
1	B	661	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	485/499 (97%)	-0.21	7 (1%) 75 71	43, 74, 120, 217	10 (2%)
1	B	486/499 (97%)	-0.02	13 (2%) 54 49	52, 94, 144, 216	8 (1%)
2	G	17/17 (100%)	-0.68	0 100 100	58, 66, 119, 157	0
2	I	16/17 (94%)	-0.76	0 100 100	46, 55, 81, 89	0
3	H	17/17 (100%)	-0.05	0 100 100	81, 91, 129, 140	0
3	J	16/17 (94%)	-0.37	0 100 100	65, 74, 88, 93	0
All	All	1037/1066 (97%)	-0.14	20 (1%) 66 62	43, 83, 137, 217	18 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	ALA	6.8
1	B	699	THR	4.8
1	B	636	ALA	4.5
1	B	697	ALA	4.3
1	B	491	HIS	3.8
1	B	237	ALA	3.4
1	B	698	LEU	3.1
1	A	471	GLY	2.9
1	B	472	GLY	2.9
1	B	495	PRO	2.8
1	A	458	GLY	2.6
1	B	706	LEU	2.4
1	A	456	ALA	2.4
1	A	546	GLU	2.4
1	A	695	LEU	2.3
1	A	557	GLN	2.2
1	B	616	VAL	2.2
1	B	662	GLY	2.1
1	B	628	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	459	LEU	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.