



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:36 AM UTC

PDB ID : 1WZX / pdb_00001wzx
Title : Crystal Structure of Family 30 Carbohydrate Binding Module.
Authors : Horiguchi, Y.; Kono, M.; Suzuki, A.; Yamane, T.; Arai, M.; Sakka, K.; Omiya, K.
Deposited on : 2005-03-10
Resolution : 3.52 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

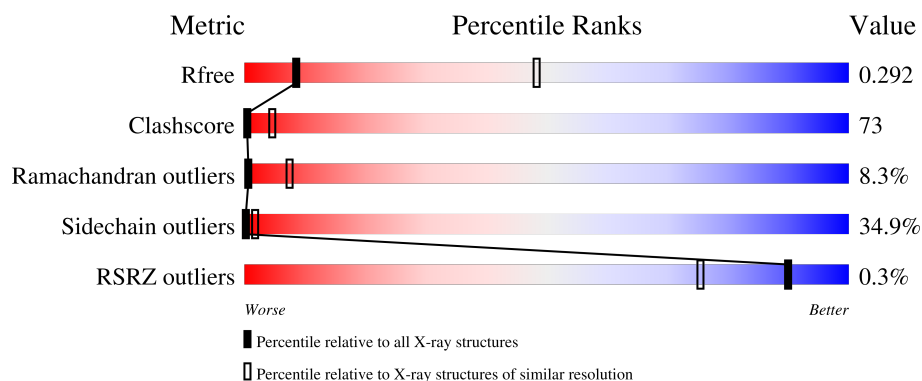
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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 $\leq 5\%$. 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	205	
1	B	205	
1	C	205	
1	D	205	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5564 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.

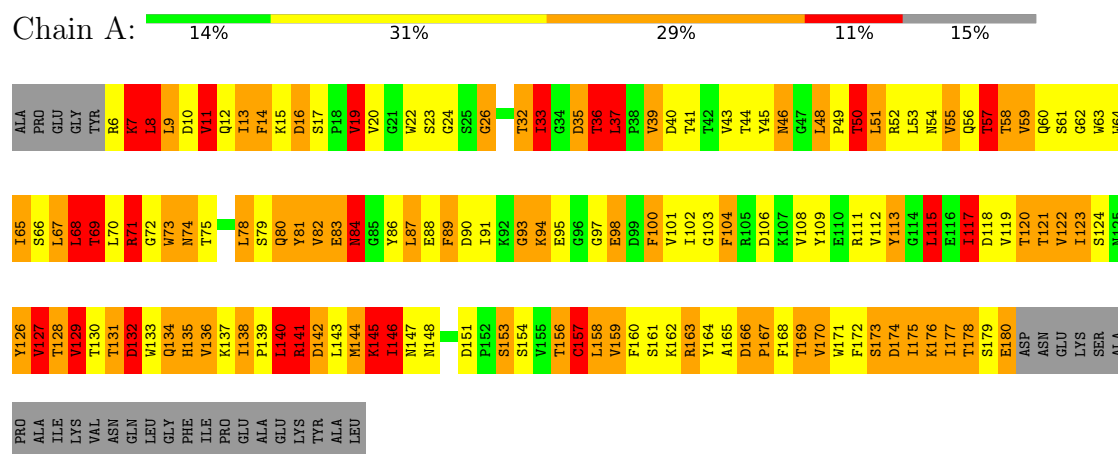
- Molecule 1 is a protein called COG3291: FOG: PKD repeat.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1404	904	227	270	3			
1	B	174	Total	C	N	O	S	0	0	0
			1392	896	222	271	3			
1	C	173	Total	C	N	O	S	0	0	0
			1384	892	221	268	3			
1	D	173	Total	C	N	O	S	0	0	0
			1384	892	221	268	3			

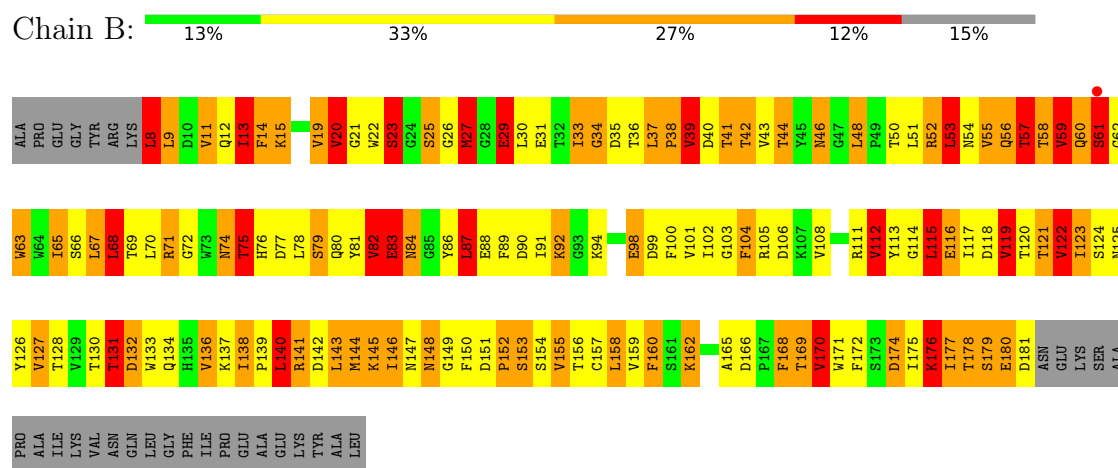
3 Residue-property plots

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.

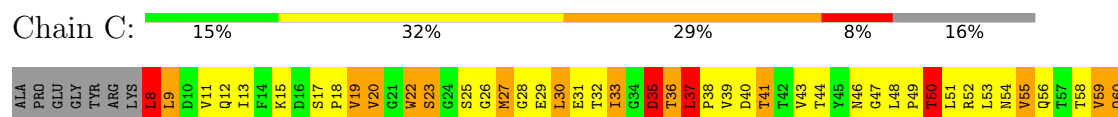
- Molecule 1: COG3291: FOG: PKD repeat

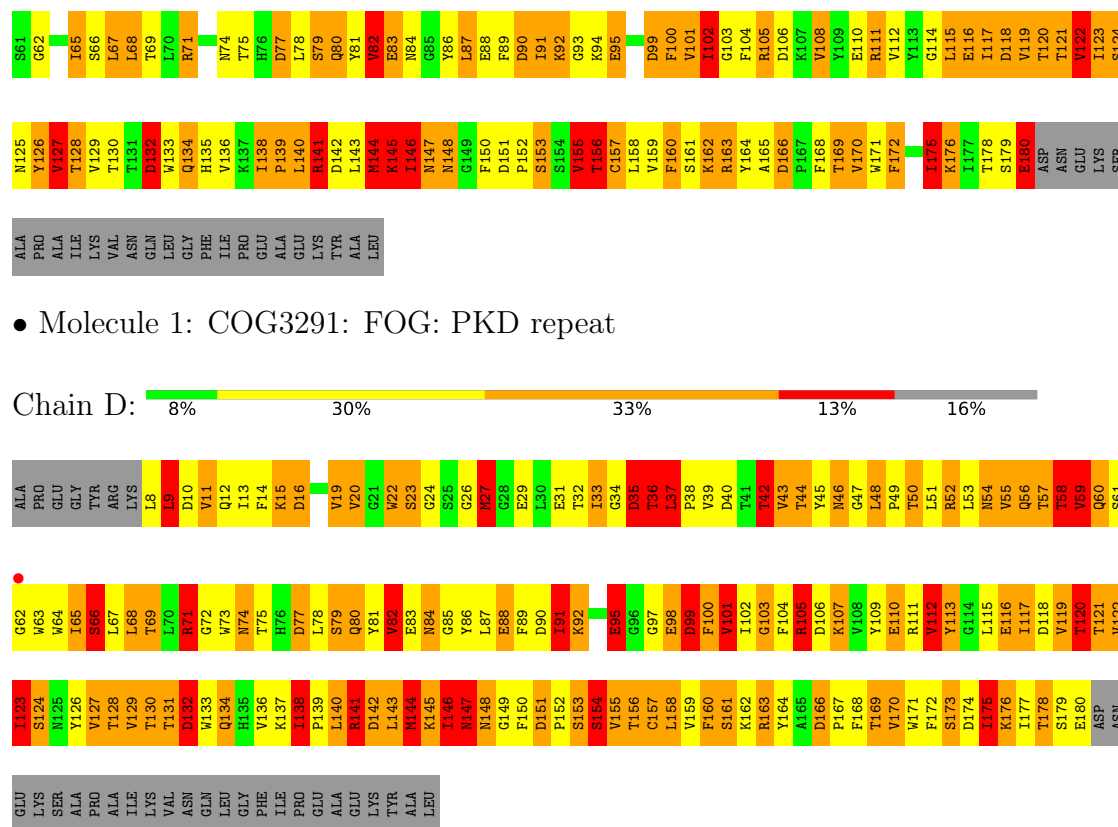


- Molecule 1: COG3291: FOG: PKD repeat



- Molecule 1: COG3291: FOG: PKD repeat





● Molecule 1: COG3291: FOG: PKD repeat

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.11Å 121.11Å 122.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.83 – 3.52 20.83 – 3.52	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.83-3.52) 95.7 (20.83-3.52)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.294 0.205 , 0.292	Depositor DCC
R_{free} test set	626 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.145 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5564	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	2.17	56/1438 (3.9%)	2.04	52/1960 (2.7%)
1	B	2.04	31/1426 (2.2%)	1.96	61/1946 (3.1%)
1	C	1.99	35/1418 (2.5%)	1.93	46/1935 (2.4%)
1	D	2.00	31/1418 (2.2%)	1.97	60/1935 (3.1%)
All	All	2.05	153/5700 (2.7%)	1.97	219/7776 (2.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	5
1	D	0	3
All	All	0	17

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	58	THR	CA-CB	12.43	1.68	1.53
1	D	59	VAL	CA-CB	11.48	1.70	1.54
1	A	41	THR	CA-CB	10.72	1.70	1.53
1	A	19	VAL	CA-C	-10.44	1.40	1.52
1	B	13	ILE	CA-CB	-10.29	1.42	1.54
1	C	138	ILE	CA-CB	-9.73	1.42	1.54
1	B	44	THR	CA-CB	9.21	1.69	1.53
1	C	122	VAL	CA-CB	-9.18	1.43	1.54
1	B	39	VAL	CA-CB	-9.09	1.43	1.54
1	A	173	SER	CA-C	-8.99	1.41	1.52
1	B	177	ILE	CA-CB	-8.97	1.43	1.54
1	C	160	PHE	CA-C	-8.95	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	LEU	CA-C	-8.89	1.45	1.52
1	A	19	VAL	CA-CB	-8.81	1.43	1.54
1	A	145	LYS	CA-C	8.79	1.65	1.53
1	C	172	PHE	CA-C	-8.61	1.42	1.52
1	C	22	TRP	CA-C	-8.59	1.41	1.52
1	C	99	ASP	CB-CG	8.49	1.73	1.52
1	B	59	VAL	CA-CB	8.41	1.65	1.54
1	A	104	PHE	CA-C	-8.26	1.42	1.52
1	D	112	VAL	CA-C	-8.25	1.44	1.52
1	B	176	LYS	CA-C	-8.22	1.42	1.52
1	A	129	VAL	CA-CB	-8.21	1.44	1.54
1	A	175	ILE	CA-CB	-8.21	1.44	1.54
1	C	128	THR	CA-CB	8.17	1.66	1.53
1	A	53	LEU	C-O	-8.15	1.14	1.23
1	D	155	VAL	CA-CB	-8.11	1.45	1.54
1	B	90	ASP	CA-C	-7.97	1.42	1.52
1	A	159	VAL	CA-CB	-7.85	1.44	1.54
1	A	100	PHE	CA-CB	-7.75	1.43	1.53
1	A	8	LEU	N-CA	7.74	1.55	1.46
1	A	117	ILE	CA-CB	-7.72	1.42	1.54
1	D	147	ASN	N-CA	7.71	1.56	1.46
1	D	156	THR	CA-C	-7.70	1.43	1.52
1	A	53	LEU	CA-C	-7.69	1.43	1.53
1	D	138	ILE	CA-C	-7.69	1.46	1.53
1	A	68	LEU	CA-C	-7.66	1.43	1.52
1	D	71	ARG	CA-CB	7.64	1.58	1.53
1	B	160	PHE	CA-C	-7.53	1.43	1.52
1	A	65	ILE	CA-CB	-7.51	1.44	1.55
1	A	104	PHE	N-CA	-7.45	1.36	1.46
1	B	19	VAL	CA-CB	-7.42	1.45	1.54
1	A	19	VAL	N-CA	-6.96	1.38	1.46
1	D	68	LEU	CA-C	-6.83	1.44	1.52
1	D	66	SER	N-CA	-6.78	1.38	1.46
1	B	136	VAL	CA-CB	-6.75	1.48	1.55
1	C	146	ILE	N-CA	6.64	1.54	1.46
1	C	175	ILE	N-CA	-6.63	1.38	1.46
1	C	68	LEU	CA-C	-6.56	1.44	1.52
1	A	7	LYS	N-CA	6.48	1.54	1.46
1	C	138	ILE	CA-C	-6.46	1.47	1.53
1	D	143	LEU	CA-C	-6.46	1.44	1.52
1	A	69	THR	CA-C	-6.43	1.44	1.53
1	A	36	THR	CA-CB	-6.38	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	144	MET	CB-CG	6.36	1.71	1.52
1	C	59	VAL	CA-CB	6.32	1.60	1.53
1	C	175	ILE	CA-C	-6.31	1.45	1.52
1	C	35	ASP	CB-CG	6.30	1.67	1.52
1	C	93	GLY	N-CA	6.29	1.51	1.44
1	C	175	ILE	CA-CB	-6.26	1.46	1.54
1	A	71	ARG	CA-CB	6.22	1.57	1.53
1	C	22	TRP	N-CA	-6.17	1.38	1.46
1	D	101	VAL	CA-CB	-6.16	1.44	1.55
1	C	165	ALA	CA-C	6.14	1.60	1.52
1	C	116	GLU	N-CA	-6.12	1.38	1.46
1	B	13	ILE	CA-C	-6.09	1.46	1.52
1	C	117	ILE	CA-CB	-6.08	1.45	1.54
1	B	71	ARG	CA-CB	6.05	1.57	1.53
1	C	155	VAL	N-CA	-6.04	1.39	1.46
1	D	22	TRP	N-CA	-6.04	1.38	1.46
1	C	138	ILE	N-CA	-6.04	1.40	1.46
1	A	167	PRO	N-CA	-6.03	1.39	1.47
1	A	7	LYS	CG-CD	6.03	1.70	1.52
1	C	27	MET	CA-C	6.02	1.60	1.52
1	B	113	TYR	N-CA	-5.99	1.39	1.46
1	C	102	ILE	CA-CB	-5.99	1.46	1.55
1	D	169	THR	CA-CB	-5.95	1.43	1.53
1	A	57	THR	C-O	-5.95	1.16	1.24
1	A	122	VAL	CA-CB	-5.91	1.47	1.54
1	A	145	LYS	CB-CG	5.86	1.70	1.52
1	A	104	PHE	CA-CB	-5.79	1.43	1.53
1	C	50	THR	CA-CB	-5.74	1.42	1.54
1	C	156	THR	CA-CB	5.73	1.62	1.53
1	A	17	SER	N-CA	5.73	1.52	1.46
1	A	83	GLU	CG-CD	5.70	1.66	1.52
1	D	148	ASN	CA-C	-5.68	1.44	1.52
1	A	44	THR	CA-C	5.68	1.60	1.53
1	D	138	ILE	CA-CB	-5.65	1.47	1.54
1	D	145	LYS	CG-CD	5.64	1.69	1.52
1	A	126	TYR	CA-C	-5.62	1.45	1.52
1	D	144	MET	CG-SD	5.61	1.94	1.80
1	D	42	THR	CA-C	5.60	1.60	1.52
1	A	33	ILE	C-O	5.60	1.29	1.24
1	B	98	GLU	CA-C	-5.59	1.45	1.52
1	D	175	ILE	CA-CB	-5.59	1.47	1.54
1	A	100	PHE	CB-CG	-5.57	1.37	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	ARG	CA-C	-5.57	1.47	1.53
1	B	170	VAL	CA-CB	-5.56	1.49	1.55
1	A	7	LYS	CA-C	5.55	1.60	1.52
1	B	104	PHE	CA-C	-5.54	1.46	1.52
1	B	61	SER	CA-CB	5.52	1.62	1.53
1	C	112	VAL	CA-CB	5.51	1.60	1.55
1	A	141	ARG	CB-CG	5.50	1.69	1.52
1	B	13	ILE	N-CA	-5.50	1.39	1.46
1	A	7	LYS	CB-CG	5.48	1.68	1.52
1	D	9	LEU	N-CA	5.48	1.53	1.46
1	B	112	VAL	CA-CB	5.46	1.61	1.54
1	B	119	VAL	CA-CB	-5.46	1.47	1.54
1	D	115	LEU	CA-C	-5.46	1.47	1.53
1	A	33	ILE	CA-C	-5.44	1.46	1.52
1	B	58	THR	N-CA	-5.43	1.39	1.46
1	D	22	TRP	CA-C	-5.42	1.45	1.52
1	A	104	PHE	C-O	-5.42	1.17	1.23
1	C	128	THR	CA-C	5.39	1.59	1.52
1	A	57	THR	CA-C	-5.36	1.45	1.52
1	B	178	THR	CA-C	-5.35	1.46	1.52
1	C	145	LYS	CA-C	5.35	1.59	1.52
1	B	15	LYS	CG-CD	5.34	1.68	1.52
1	A	41	THR	CB-CG2	5.33	1.70	1.52
1	A	11	VAL	N-CA	5.32	1.53	1.46
1	B	53	LEU	CA-C	-5.31	1.46	1.53
1	D	15	LYS	CG-CD	5.30	1.68	1.52
1	D	119	VAL	CA-CB	5.30	1.60	1.54
1	A	39	VAL	CA-CB	-5.29	1.48	1.54
1	A	153	SER	N-CA	-5.29	1.39	1.46
1	A	98	GLU	C-O	-5.26	1.17	1.23
1	A	74	ASN	CA-C	-5.26	1.46	1.52
1	A	132	ASP	CA-C	-5.26	1.46	1.52
1	A	145	LYS	CG-CD	5.26	1.68	1.52
1	B	169	THR	CA-CB	-5.25	1.45	1.54
1	D	119	VAL	C-O	5.25	1.29	1.24
1	D	154	SER	CA-C	-5.23	1.46	1.53
1	C	80	GLN	CA-C	5.23	1.59	1.52
1	C	146	ILE	CA-C	5.23	1.59	1.52
1	A	43	VAL	CA-C	-5.20	1.48	1.53
1	A	73	TRP	CA-C	-5.20	1.46	1.52
1	C	147	ASN	C-O	5.18	1.30	1.24
1	B	87	LEU	N-CA	-5.18	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	LYS	CD-CE	5.16	1.68	1.52
1	B	122	VAL	N-CA	-5.15	1.40	1.46
1	C	95	GLU	CA-CB	5.14	1.60	1.53
1	B	168	PHE	N-CA	-5.11	1.40	1.46
1	D	128	THR	CA-C	5.11	1.59	1.52
1	A	135	HIS	CA-C	5.08	1.59	1.53
1	B	174	ASP	CB-CG	5.07	1.64	1.52
1	D	42	THR	CA-CB	5.07	1.62	1.53
1	A	113	TYR	CA-C	5.06	1.59	1.52
1	C	172	PHE	CA-CB	-5.06	1.45	1.54
1	B	27	MET	CA-C	5.06	1.59	1.52
1	D	97	GLY	N-CA	5.05	1.52	1.45
1	B	79	SER	CA-C	5.05	1.59	1.52
1	C	146	ILE	CA-CB	5.03	1.61	1.54
1	A	174	ASP	CB-CG	5.00	1.64	1.52

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	VAL	CB-CA-C	-12.72	96.92	111.55
1	B	13	ILE	N-CA-C	-12.50	101.06	111.81
1	A	166	ASP	CA-C-N	11.82	134.61	119.84
1	A	166	ASP	C-N-CA	11.82	134.61	119.84
1	D	157	CYS	N-CA-C	11.72	125.72	108.60
1	B	19	VAL	CB-CA-C	-10.89	95.45	111.68
1	A	8	LEU	N-CA-C	10.75	126.91	109.59
1	B	146	ILE	CB-CA-C	-10.59	98.33	110.41
1	D	138	ILE	CB-CA-C	-9.72	99.67	110.85
1	B	113	TYR	N-CA-C	-9.44	102.97	112.97
1	C	138	ILE	CA-C-N	9.38	131.57	119.84
1	C	138	ILE	C-N-CA	9.38	131.57	119.84
1	A	48	LEU	CA-C-N	9.12	129.06	120.03
1	A	48	LEU	C-N-CA	9.12	129.06	120.03
1	A	60	GLN	N-CA-CB	-9.05	96.82	110.12
1	A	138	ILE	CA-C-N	8.74	130.76	119.84
1	A	138	ILE	C-N-CA	8.74	130.76	119.84
1	B	132	ASP	N-CA-C	8.58	123.42	108.75
1	A	157	CYS	N-CA-C	8.57	121.11	108.60
1	A	37	LEU	CA-C-N	8.43	128.45	119.76
1	A	37	LEU	C-N-CA	8.43	128.45	119.76
1	C	50	THR	CB-CA-C	-8.21	92.96	109.79
1	A	153	SER	N-CA-C	-8.18	102.32	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	CYS	N-CA-C	8.13	120.49	108.14
1	C	35	ASP	N-CA-C	-7.85	103.65	113.23
1	D	138	ILE	CA-C-N	7.84	128.29	119.83
1	D	138	ILE	C-N-CA	7.84	128.29	119.83
1	D	91	ILE	N-CA-C	7.79	118.95	108.27
1	D	156	THR	CB-CA-C	-7.76	96.61	109.65
1	B	108	VAL	CB-CA-C	-7.70	97.09	110.65
1	C	13	ILE	N-CA-C	-7.68	104.31	111.45
1	C	37	LEU	CA-C-N	7.67	127.44	119.76
1	C	37	LEU	C-N-CA	7.67	127.44	119.76
1	A	81	TYR	N-CA-C	7.56	119.60	111.36
1	A	60	GLN	CA-C-N	7.54	130.24	120.44
1	A	60	GLN	C-N-CA	7.54	130.24	120.44
1	A	11	VAL	N-CA-C	7.51	118.71	107.75
1	C	128	THR	CB-CA-C	7.49	122.32	109.51
1	D	103	GLY	N-CA-C	7.48	120.17	110.45
1	D	52	ARG	N-CA-C	7.44	120.80	108.96
1	D	59	VAL	CA-C-N	-7.38	110.37	122.54
1	D	59	VAL	C-N-CA	-7.38	110.37	122.54
1	C	105	ARG	N-CA-C	-7.37	98.21	109.85
1	A	19	VAL	CB-CA-C	-7.35	99.64	110.81
1	D	132	ASP	N-CA-C	7.31	120.31	108.76
1	C	175	ILE	N-CA-C	-7.31	97.05	108.23
1	D	63	TRP	N-CA-C	7.21	121.08	108.75
1	B	75	THR	CB-CA-C	-7.16	98.73	109.90
1	A	178	THR	CB-CA-C	-7.09	94.56	109.38
1	D	166	ASP	CA-C-N	7.09	127.13	119.90
1	D	166	ASP	C-N-CA	7.09	127.13	119.90
1	A	127	VAL	CB-CA-C	-7.07	101.97	111.80
1	B	146	ILE	N-CA-CB	7.06	121.52	112.34
1	C	129	VAL	N-CA-C	7.03	118.41	108.36
1	B	76	HIS	N-CA-C	-6.94	98.61	109.72
1	B	127	VAL	N-CA-C	6.92	118.32	108.42
1	B	166	ASP	CA-C-N	6.89	127.28	119.83
1	B	166	ASP	C-N-CA	6.89	127.28	119.83
1	A	103	GLY	N-CA-C	6.86	121.77	111.42
1	A	122	VAL	N-CA-CB	-6.85	103.19	111.00
1	C	60	GLN	N-CA-C	6.82	122.44	113.30
1	A	126	TYR	N-CA-C	-6.77	104.92	113.72
1	A	11	VAL	N-CA-CB	6.76	120.42	111.64
1	C	59	VAL	CA-C-N	-6.72	112.07	122.49
1	C	59	VAL	C-N-CA	-6.72	112.07	122.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	ILE	CB-CA-C	-6.70	100.30	111.29
1	B	122	VAL	CB-CA-C	6.67	120.77	110.83
1	D	153	SER	N-CA-C	-6.62	104.83	113.17
1	B	9	LEU	CA-CB-CG	6.57	139.31	116.30
1	B	52	ARG	N-CA-C	6.57	119.44	108.20
1	B	116	GLU	N-CA-C	-6.57	99.02	109.59
1	A	11	VAL	CB-CA-C	-6.55	101.47	110.77
1	D	117	ILE	CB-CA-C	-6.55	101.47	110.90
1	D	166	ASP	N-CA-C	6.54	117.90	109.72
1	A	59	VAL	CA-C-N	6.54	129.04	120.28
1	A	59	VAL	C-N-CA	6.54	129.04	120.28
1	D	27	MET	CB-CG-SD	-6.53	93.10	112.70
1	B	87	LEU	N-CA-C	-6.50	100.42	110.10
1	C	127	VAL	N-CA-C	6.45	116.91	107.75
1	D	69	THR	CB-CA-C	-6.44	97.07	110.40
1	C	112	VAL	CB-CA-C	-6.42	104.22	111.80
1	D	144	MET	CB-CG-SD	6.39	131.87	112.70
1	A	13	ILE	N-CA-C	-6.35	104.96	110.74
1	A	67	LEU	CB-CG-CD1	-6.33	91.71	110.70
1	B	112	VAL	N-CA-C	6.31	117.23	111.81
1	C	121	THR	N-CA-C	6.23	118.03	109.18
1	A	109	TYR	CA-C-N	6.17	128.83	120.38
1	A	109	TYR	C-N-CA	6.17	128.83	120.38
1	B	33	ILE	CB-CA-C	-6.14	101.54	110.63
1	C	68	LEU	CA-CB-CG	-6.13	94.84	116.30
1	C	92	LYS	N-CA-C	-6.13	100.17	109.85
1	D	100	PHE	CA-C-N	-6.10	113.86	122.34
1	D	100	PHE	C-N-CA	-6.10	113.86	122.34
1	A	93	GLY	CA-C-N	-6.08	111.65	120.29
1	A	93	GLY	C-N-CA	-6.08	111.65	120.29
1	C	180	GLU	CB-CA-C	-5.98	98.73	110.10
1	C	46	ASN	N-CA-C	5.97	118.49	111.02
1	A	9	LEU	N-CA-C	5.95	119.78	110.32
1	B	38	PRO	CA-C-N	-5.95	115.42	123.10
1	B	38	PRO	C-N-CA	-5.95	115.42	123.10
1	B	53	LEU	CA-C-N	-5.94	113.10	122.73
1	B	53	LEU	C-N-CA	-5.94	113.10	122.73
1	C	170	VAL	CB-CA-C	-5.89	100.20	110.38
1	D	60	GLN	N-CA-CB	5.87	119.18	110.49
1	D	146	ILE	CB-CA-C	-5.87	101.66	111.29
1	A	68	LEU	N-CA-C	-5.86	99.85	109.40
1	D	58	THR	CB-CA-C	5.86	120.47	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	VAL	CB-CA-C	-5.84	102.63	111.33
1	B	68	LEU	N-CA-C	-5.81	99.04	108.52
1	D	9	LEU	N-CA-C	5.81	119.39	110.20
1	D	48	LEU	CA-C-N	5.81	126.62	120.11
1	D	48	LEU	C-N-CA	5.81	126.62	120.11
1	C	120	THR	CB-CA-C	-5.81	97.29	110.07
1	B	166	ASP	N-CA-C	5.79	116.96	109.72
1	A	60	GLN	N-CA-C	5.79	117.59	111.28
1	C	132	ASP	N-CA-C	5.78	118.07	108.99
1	D	68	LEU	N-CA-C	-5.77	99.12	108.52
1	B	29	GLU	N-CA-CB	-5.74	101.47	110.30
1	B	11	VAL	N-CA-C	5.73	116.12	107.75
1	C	100	PHE	CA-C-N	-5.71	114.40	122.34
1	C	100	PHE	C-N-CA	-5.71	114.40	122.34
1	A	166	ASP	N-CA-C	5.71	117.89	109.62
1	D	15	LYS	N-CA-C	-5.70	104.49	112.12
1	B	48	LEU	N-CA-C	5.68	117.05	109.83
1	C	95	GLU	N-CA-C	5.68	117.11	110.41
1	B	37	LEU	CA-C-N	5.66	126.10	119.99
1	B	37	LEU	C-N-CA	5.66	126.10	119.99
1	B	112	VAL	CB-CA-C	-5.66	105.04	111.55
1	D	37	LEU	CA-C-N	5.65	126.09	119.99
1	D	37	LEU	C-N-CA	5.65	126.09	119.99
1	B	63	TRP	N-CA-C	5.65	117.70	108.55
1	B	92	LYS	N-CA-C	-5.63	101.20	109.81
1	D	23	SER	N-CA-C	-5.61	98.84	110.80
1	A	32	THR	CB-CA-C	-5.61	99.62	109.71
1	A	69	THR	CB-CA-C	-5.60	100.76	110.45
1	C	144	MET	CB-CG-SD	5.60	129.50	112.70
1	B	168	PHE	N-CA-CB	-5.58	102.86	111.46
1	A	33	ILE	N-CA-C	-5.58	99.47	107.78
1	A	141	ARG	CA-CB-CG	5.58	125.26	114.10
1	B	82	VAL	CA-C-N	5.58	132.19	121.54
1	B	82	VAL	C-N-CA	5.58	132.19	121.54
1	C	20	VAL	N-CA-CB	5.57	116.60	110.53
1	B	34	GLY	CA-C-N	-5.57	115.01	124.31
1	B	34	GLY	C-N-CA	-5.57	115.01	124.31
1	D	57	THR	CB-CA-C	-5.57	104.40	113.37
1	C	38	PRO	CB-CA-C	-5.57	103.81	111.21
1	C	180	GLU	N-CA-C	5.57	126.59	111.00
1	B	9	LEU	N-CA-C	5.56	119.30	109.96
1	C	17	SER	CA-C-N	5.54	125.48	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	SER	C-N-CA	5.54	125.48	119.78
1	B	83	GLU	N-CA-CB	-5.52	101.16	110.49
1	A	50	THR	CB-CA-C	-5.51	100.56	110.36
1	D	120	THR	CB-CA-C	-5.50	97.35	109.56
1	B	138	ILE	CB-CA-C	-5.50	104.53	110.85
1	C	82	VAL	CB-CA-C	-5.48	102.30	111.29
1	B	9	LEU	CB-CA-C	-5.48	100.49	109.53
1	C	30	LEU	N-CA-C	5.47	117.62	109.25
1	B	56	GLN	N-CA-C	5.46	122.44	110.80
1	D	36	THR	N-CA-CB	5.45	118.83	110.70
1	C	92	LYS	CA-C-N	5.45	126.26	121.58
1	C	92	LYS	C-N-CA	5.45	126.26	121.58
1	B	60	GLN	N-CA-C	5.42	119.89	113.28
1	A	58	THR	CB-CA-C	5.42	118.68	109.80
1	A	169	THR	CB-CA-C	-5.41	99.75	111.11
1	B	115	LEU	CA-C-N	-5.41	115.09	122.93
1	B	115	LEU	C-N-CA	-5.41	115.09	122.93
1	B	122	VAL	N-CA-C	-5.41	100.60	108.17
1	B	176	LYS	CB-CA-C	-5.38	98.77	109.79
1	B	128	THR	CA-C-N	-5.35	116.19	123.10
1	B	128	THR	C-N-CA	-5.35	116.19	123.10
1	D	156	THR	OG1-CB-CG2	5.34	119.98	109.30
1	C	35	ASP	CB-CA-C	5.34	120.17	111.26
1	C	8	LEU	N-CA-C	5.33	125.91	111.00
1	C	160	PHE	CB-CA-C	-5.32	101.94	110.14
1	D	13	ILE	N-CA-C	-5.31	105.67	110.82
1	B	23	SER	N-CA-C	-5.30	99.51	110.80
1	A	156	THR	CB-CA-C	-5.30	101.12	109.34
1	D	35	ASP	CA-C-N	-5.30	113.56	123.05
1	D	35	ASP	C-N-CA	-5.30	113.56	123.05
1	A	129	VAL	N-CA-C	5.26	115.88	108.36
1	B	180	GLU	N-CA-C	5.25	121.97	110.80
1	A	167	PRO	CB-CA-C	-5.21	102.96	111.56
1	D	86	TYR	CB-CA-C	-5.20	103.56	110.79
1	B	131	THR	CB-CA-C	-5.20	100.07	110.42
1	C	117	ILE	N-CA-C	5.20	117.10	108.99
1	D	129	VAL	N-CA-C	5.20	115.79	108.36
1	D	99	ASP	N-CA-C	5.20	117.29	109.23
1	D	166	ASP	CA-C-O	5.19	123.92	119.66
1	C	139	PRO	CB-CA-C	-5.19	103.00	111.56
1	D	44	THR	N-CA-CB	5.17	117.52	110.38
1	B	59	VAL	CA-C-N	-5.17	112.44	122.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	VAL	C-N-CA	-5.17	112.44	122.06
1	A	159	VAL	N-CA-C	5.16	115.17	108.35
1	D	105	ARG	N-CA-C	-5.16	102.14	110.14
1	A	126	TYR	CA-C-N	-5.15	115.06	121.96
1	A	126	TYR	C-N-CA	-5.15	115.06	121.96
1	D	155	VAL	CB-CA-C	-5.14	104.18	111.28
1	C	127	VAL	CB-CA-C	-5.14	104.16	111.40
1	A	59	VAL	N-CA-CB	-5.13	102.76	111.23
1	D	138	ILE	N-CA-CB	5.12	117.84	111.39
1	B	12	GLN	CA-C-N	-5.12	116.31	122.35
1	B	12	GLN	C-N-CA	-5.12	116.31	122.35
1	B	153	SER	N-CA-C	-5.10	106.30	112.88
1	D	160	PHE	CA-C-N	-5.07	114.29	122.81
1	D	160	PHE	C-N-CA	-5.07	114.29	122.81
1	A	146	ILE	CB-CA-C	-5.07	102.98	111.29
1	D	120	THR	N-CA-C	5.06	117.08	109.23
1	B	57	THR	N-CA-CB	5.05	119.14	110.65
1	D	147	ASN	N-CA-C	5.05	121.56	110.80
1	C	87	LEU	N-CA-C	-5.05	102.73	110.30
1	D	57	THR	N-CA-C	5.04	118.37	109.80
1	D	151	ASP	N-CA-C	5.03	118.45	108.59
1	D	54	ASN	N-CA-C	5.03	116.71	108.52
1	A	33	ILE	CB-CA-C	-5.02	103.29	110.12
1	D	110	GLU	CA-C-N	5.02	127.98	120.95
1	D	110	GLU	C-N-CA	5.02	127.98	120.95
1	C	120	THR	N-CA-C	5.01	116.81	109.24
1	B	30	LEU	CB-CA-C	-5.00	101.69	109.84
1	D	40	ASP	N-CA-C	5.00	116.91	108.96

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ASP	Peptide
1	A	140	LEU	Peptide
1	A	145	LYS	Peptide
1	A	7	LYS	Peptide
1	B	140	LEU	Peptide
1	B	145	LYS	Peptide
1	B	179	SER	Peptide
1	B	60	GLN	Peptide
1	B	8	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	120	THR	Peptide
1	C	145	LYS	Peptide
1	C	179	SER	Peptide
1	C	35	ASP	Peptide
1	C	8	LEU	Peptide
1	D	120	THR	Peptide
1	D	127	VAL	Peptide
1	D	35	ASP	Peptide

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	1404	0	1377	230	0
1	B	1392	0	1355	177	0
1	C	1384	0	1351	181	0
1	D	1384	0	1351	220	0
All	All	5564	0	5434	802	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 73.

All (802) 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:D:140:LEU:HD12	1:D:144:MET:CE	1.43	1.46
1:A:89:PHE:CD1	1:A:91:ILE:HD11	1.68	1.27
1:A:89:PHE:CE1	1:A:91:ILE:HD11	1.71	1.26
1:D:140:LEU:CD1	1:D:144:MET:HE1	1.69	1.23
1:D:98:GLU:OE1	1:D:168:PHE:HB3	1.48	1.13
1:C:54:ASN:HA	1:C:169:THR:HG23	1.26	1.12
1:A:50:THR:HG22	1:A:172:PHE:O	1.46	1.12
1:D:140:LEU:CD1	1:D:144:MET:CE	2.24	1.12
1:B:59:VAL:HG23	1:B:62:GLY:H	1.16	1.11
1:A:71:ARG:HG2	1:A:71:ARG:HH11	0.94	1.10
1:A:169:THR:HG22	1:A:170:VAL:H	1.00	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:SER:HB2	1:B:29:GLU:HG3	1.33	1.10
1:A:57:THR:HG23	1:A:58:THR:N	1.60	1.08
1:A:123:ILE:HD13	1:A:123:ILE:H	0.98	1.08
1:D:8:LEU:HD12	1:D:9:LEU:H	1.16	1.06
1:B:111:ARG:NH2	1:B:117:ILE:HD13	1.70	1.06
1:C:146:ILE:O	1:C:148:ASN:N	1.89	1.05
1:C:92:LYS:HD3	1:C:133:TRP:NE1	1.70	1.05
1:D:144:MET:HG3	1:D:150:PHE:HE2	1.17	1.05
1:A:140:LEU:HD12	1:A:144:MET:HE3	1.37	1.03
1:B:69:THR:HA	1:B:157:CYS:HB3	1.38	1.03
1:D:10:ASP:OD2	1:D:178:THR:HG22	1.59	1.03
1:A:140:LEU:CD1	1:A:144:MET:HE3	1.89	1.02
1:B:100:PHE:H	1:B:123:ILE:CD1	1.72	1.02
1:D:169:THR:HG22	1:D:170:VAL:N	1.73	1.02
1:A:127:VAL:HG12	1:A:128:THR:O	1.59	1.01
1:C:50:THR:HG22	1:C:172:PHE:O	1.61	1.01
1:C:54:ASN:CA	1:C:169:THR:HG23	1.91	1.01
1:D:48:LEU:HD13	1:D:49:PRO:HD2	1.42	0.99
1:A:16:ASP:HB3	1:A:48:LEU:HD23	1.43	0.99
1:D:50:THR:HG22	1:D:172:PHE:O	1.62	0.99
1:A:69:THR:HA	1:A:157:CYS:HB3	1.39	0.99
1:A:169:THR:HG22	1:A:170:VAL:N	1.67	0.99
1:A:57:THR:HG23	1:A:58:THR:H	1.15	0.98
1:B:82:VAL:HG12	1:B:83:GLU:N	1.77	0.98
1:A:6:ARG:HG2	1:A:8:LEU:HD21	1.42	0.98
1:C:20:VAL:O	1:C:69:THR:HG23	1.63	0.98
1:D:144:MET:HG3	1:D:150:PHE:CE2	1.98	0.98
1:A:123:ILE:HD13	1:A:123:ILE:N	1.75	0.97
1:D:140:LEU:HD12	1:D:144:MET:HE2	1.48	0.96
1:D:100:PHE:H	1:D:123:ILE:HD11	1.31	0.95
1:C:69:THR:HA	1:C:157:CYS:HB3	1.48	0.95
1:A:123:ILE:H	1:A:123:ILE:CD1	1.80	0.94
1:D:45:TYR:O	1:D:46:ASN:HB2	1.65	0.94
1:B:87:LEU:HD12	1:B:88:GLU:N	1.83	0.93
1:D:100:PHE:H	1:D:123:ILE:CD1	1.82	0.93
1:C:59:VAL:HG11	1:C:162:LYS:HD2	1.50	0.93
1:B:54:ASN:HB2	1:B:169:THR:HG23	1.50	0.92
1:C:117:ILE:HG22	1:C:118:ASP:N	1.82	0.92
1:C:67:LEU:C	1:C:68:LEU:HD23	1.95	0.92
1:A:101:VAL:CG1	1:A:120:THR:HG23	2.00	0.92
1:C:67:LEU:O	1:C:68:LEU:HD23	1.70	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:OE1	1:A:135:HIS:CE1	2.24	0.91
1:B:77:ASP:OD1	1:B:153:SER:HB2	1.70	0.90
1:B:75:THR:HG22	1:B:154:SER:HA	1.52	0.90
1:D:82:VAL:CG1	1:D:83:GLU:N	2.36	0.89
1:D:68:LEU:O	1:D:157:CYS:HB2	1.73	0.89
1:A:169:THR:CG2	1:A:170:VAL:H	1.85	0.89
1:A:57:THR:CG2	1:A:58:THR:N	2.31	0.88
1:A:146:ILE:O	1:A:148:ASN:N	2.07	0.88
1:D:111:ARG:NH2	1:D:117:ILE:HG12	1.89	0.88
1:A:89:PHE:CE1	1:A:91:ILE:CD1	2.56	0.88
1:A:71:ARG:HG2	1:A:71:ARG:NH1	1.67	0.87
1:D:82:VAL:HG13	1:D:83:GLU:N	1.87	0.87
1:C:146:ILE:O	1:C:148:ASN:HB3	1.75	0.86
1:D:91:ILE:HD13	1:D:91:ILE:O	1.75	0.86
1:B:111:ARG:CZ	1:B:117:ILE:HD13	2.04	0.86
1:C:8:LEU:HG	1:C:9:LEU:N	1.86	0.86
1:C:119:VAL:HG22	1:C:150:PHE:CE1	2.11	0.86
1:B:69:THR:HA	1:B:157:CYS:CB	2.06	0.86
1:D:140:LEU:HD12	1:D:144:MET:HE1	0.87	0.86
1:D:169:THR:CG2	1:D:170:VAL:N	2.39	0.85
1:B:121:THR:HG21	1:B:126:TYR:HE2	1.42	0.85
1:D:8:LEU:CD1	1:D:9:LEU:HD12	2.07	0.85
1:A:15:LYS:HE2	1:A:48:LEU:HD21	1.59	0.84
1:B:25:SER:CB	1:B:29:GLU:HG3	2.07	0.84
1:C:146:ILE:C	1:C:148:ASN:H	1.84	0.84
1:D:113:TYR:H	1:D:113:TYR:HD2	1.23	0.84
1:D:144:MET:CG	1:D:150:PHE:HE2	1.89	0.84
1:A:175:ILE:HD12	1:A:175:ILE:N	1.90	0.84
1:D:69:THR:HA	1:D:157:CYS:HB3	1.59	0.83
1:D:130:THR:OG1	1:D:132:ASP:HB2	1.78	0.83
1:C:23:SER:HB3	1:C:66:SER:OG	1.76	0.83
1:D:44:THR:OG1	1:D:45:TYR:N	2.06	0.83
1:C:111:ARG:NH2	1:C:117:ILE:HD12	1.93	0.83
1:B:99:ASP:OD1	1:B:123:ILE:HD13	1.79	0.82
1:A:100:PHE:H	1:A:123:ILE:HD11	1.43	0.82
1:B:143:LEU:O	1:B:145:LYS:N	2.12	0.81
1:D:100:PHE:N	1:D:123:ILE:HD11	1.95	0.81
1:B:121:THR:HG21	1:B:126:TYR:CE2	2.16	0.81
1:B:143:LEU:N	1:B:143:LEU:HD13	1.95	0.81
1:D:20:VAL:O	1:D:69:THR:HG23	1.80	0.81
1:C:54:ASN:HB2	1:C:169:THR:CG2	2.11	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASP:HA	1:D:123:ILE:HD11	1.62	0.81
1:A:16:ASP:CB	1:A:48:LEU:HD23	2.09	0.81
1:A:179:SER:OG	1:A:180:GLU:N	2.11	0.81
1:B:13:ILE:HG22	1:B:14:PHE:N	1.96	0.80
1:A:143:LEU:O	1:A:145:LYS:N	2.13	0.80
1:B:59:VAL:HG23	1:B:62:GLY:N	1.95	0.80
1:B:100:PHE:H	1:B:123:ILE:HD11	1.44	0.80
1:C:29:GLU:OE2	1:C:29:GLU:N	2.14	0.80
1:B:143:LEU:N	1:B:143:LEU:CD1	2.44	0.79
1:C:43:VAL:HG12	1:C:43:VAL:O	1.81	0.79
1:B:136:VAL:HG22	1:B:137:LYS:N	1.97	0.79
1:C:9:LEU:O	1:C:81:TYR:OH	1.99	0.79
1:C:54:ASN:CB	1:C:169:THR:HG23	2.12	0.79
1:C:102:ILE:HD12	1:C:160:PHE:HE2	1.48	0.79
1:C:111:ARG:HG3	1:C:114:GLY:O	1.83	0.79
1:D:91:ILE:HD13	1:D:91:ILE:C	2.07	0.79
1:A:100:PHE:O	1:A:123:ILE:CD1	2.31	0.79
1:C:55:VAL:HG13	1:C:168:PHE:H	1.48	0.79
1:C:68:LEU:O	1:C:157:CYS:HB2	1.83	0.79
1:D:59:VAL:HG23	1:D:62:GLY:H	1.48	0.78
1:C:111:ARG:HH21	1:C:117:ILE:HD12	1.49	0.78
1:B:140:LEU:O	1:B:141:ARG:C	2.25	0.78
1:D:22:TRP:CH2	1:D:24:GLY:HA3	2.18	0.78
1:C:130:THR:C	1:C:132:ASP:H	1.92	0.78
1:B:146:ILE:O	1:B:148:ASN:N	2.14	0.77
1:B:68:LEU:O	1:B:157:CYS:HB2	1.84	0.77
1:B:111:ARG:NH2	1:B:117:ILE:CD1	2.46	0.77
1:D:163:ARG:HD3	1:D:164:TYR:CE2	2.20	0.77
1:A:130:THR:C	1:A:132:ASP:H	1.93	0.77
1:A:143:LEU:C	1:A:145:LYS:H	1.87	0.77
1:D:105:ARG:HA	1:D:117:ILE:O	1.83	0.77
1:B:25:SER:HB2	1:B:29:GLU:CG	2.14	0.77
1:D:8:LEU:HD12	1:D:9:LEU:N	1.99	0.77
1:A:22:TRP:O	1:A:67:LEU:HB2	1.85	0.76
1:C:111:ARG:CG	1:C:114:GLY:O	2.33	0.76
1:B:125:ASN:O	1:D:20:VAL:HG11	1.84	0.76
1:B:82:VAL:CG1	1:B:83:GLU:N	2.48	0.76
1:B:169:THR:HG22	1:B:170:VAL:N	2.01	0.76
1:C:127:VAL:HG11	1:C:134:GLN:NE2	2.00	0.76
1:B:136:VAL:CG2	1:B:137:LYS:N	2.48	0.76
1:A:119:VAL:HG21	1:A:143:LEU:HB3	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:HD12	1:D:9:LEU:HD12	1.66	0.75
1:A:101:VAL:HG11	1:A:120:THR:HG23	1.67	0.75
1:B:143:LEU:C	1:B:145:LYS:H	1.92	0.75
1:C:92:LYS:HD3	1:C:133:TRP:CE2	2.21	0.75
1:C:117:ILE:HG22	1:C:118:ASP:H	1.48	0.75
1:D:12:GLN:NE2	1:D:175:ILE:O	2.19	0.74
1:D:55:VAL:HG13	1:D:168:PHE:H	1.52	0.74
1:D:179:SER:O	1:D:180:GLU:HG3	1.87	0.74
1:C:140:LEU:O	1:C:141:ARG:C	2.28	0.74
1:A:14:PHE:CD1	1:A:14:PHE:C	2.65	0.74
1:A:16:ASP:HB3	1:A:48:LEU:CD2	2.17	0.74
1:A:55:VAL:HG23	1:A:168:PHE:H	1.52	0.74
1:D:91:ILE:HA	1:D:133:TRP:CZ3	2.23	0.74
1:D:139:PRO:O	1:D:142:ASP:OD1	2.06	0.74
1:C:117:ILE:CG2	1:C:118:ASP:N	2.50	0.73
1:C:143:LEU:HD12	1:C:143:LEU:H	1.51	0.73
1:D:123:ILE:HG12	1:D:124:SER:H	1.53	0.73
1:C:87:LEU:HD12	1:C:104:PHE:HZ	1.53	0.73
1:A:54:ASN:HD22	1:A:55:VAL:N	1.86	0.73
1:D:95:GLU:HG2	1:D:95:GLU:O	1.89	0.73
1:B:140:LEU:HD12	1:B:144:MET:HG3	1.71	0.72
1:C:127:VAL:CG1	1:C:134:GLN:NE2	2.52	0.72
1:C:54:ASN:HA	1:C:169:THR:CG2	2.13	0.72
1:A:71:ARG:NH1	1:A:71:ARG:CG	2.51	0.72
1:B:170:VAL:HG13	1:B:171:TRP:N	2.04	0.72
1:D:169:THR:HG21	1:D:171:TRP:CH2	2.24	0.72
1:A:54:ASN:ND2	1:A:168:PHE:O	2.23	0.72
1:A:159:VAL:O	1:A:160:PHE:HD1	1.72	0.72
1:B:121:THR:HG23	1:B:122:VAL:N	2.04	0.72
1:A:100:PHE:N	1:A:100:PHE:CD2	2.52	0.71
1:A:175:ILE:N	1:A:175:ILE:CD1	2.53	0.71
1:A:90:ASP:C	1:A:91:ILE:HD12	2.15	0.71
1:C:23:SER:HB3	1:C:66:SER:CB	2.19	0.71
1:A:15:LYS:HE2	1:A:48:LEU:CD2	2.20	0.71
1:D:131:THR:HG22	1:D:131:THR:O	1.91	0.71
1:B:130:THR:C	1:B:132:ASP:H	1.98	0.71
1:C:54:ASN:HB2	1:C:169:THR:HG21	1.73	0.71
1:B:174:ASP:OD1	1:B:176:LYS:HE2	1.90	0.71
1:A:89:PHE:HB3	1:A:175:ILE:HA	1.71	0.71
1:C:92:LYS:CD	1:C:133:TRP:NE1	2.50	0.71
1:D:146:ILE:O	1:D:148:ASN:N	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:PHE:C	1:B:14:PHE:CD2	2.66	0.70
1:A:54:ASN:ND2	1:A:55:VAL:N	2.39	0.70
1:A:89:PHE:CB	1:A:175:ILE:HG13	2.21	0.70
1:C:117:ILE:CG2	1:C:118:ASP:H	2.05	0.70
1:D:69:THR:HA	1:D:157:CYS:CB	2.21	0.70
1:A:89:PHE:CD1	1:A:91:ILE:CD1	2.62	0.70
1:A:101:VAL:HG12	1:A:102:ILE:N	2.05	0.70
1:B:125:ASN:HD22	1:B:125:ASN:N	1.89	0.70
1:A:22:TRP:CH2	1:A:24:GLY:HA3	2.27	0.69
1:A:89:PHE:HE1	1:A:91:ILE:HD11	1.51	0.69
1:C:40:ASP:OD2	1:C:41:THR:N	2.25	0.69
1:C:30:LEU:HD12	1:C:31:GLU:N	2.07	0.69
1:D:91:ILE:HG12	1:D:170:VAL:HG23	1.73	0.69
1:B:54:ASN:HD22	1:B:55:VAL:N	1.91	0.69
1:B:88:GLU:HB3	1:B:137:LYS:HG2	1.74	0.69
1:C:121:THR:OG1	1:C:122:VAL:N	2.25	0.69
1:D:82:VAL:CG1	1:D:83:GLU:H	2.06	0.69
1:A:82:VAL:HG12	1:A:83:GLU:N	2.06	0.69
1:C:54:ASN:CB	1:C:169:THR:CG2	2.69	0.69
1:A:22:TRP:CZ3	1:A:24:GLY:N	2.61	0.69
1:B:105:ARG:HA	1:B:117:ILE:O	1.92	0.68
1:B:143:LEU:HD13	1:B:143:LEU:H	1.55	0.68
1:D:140:LEU:CD1	1:D:144:MET:HE2	2.10	0.68
1:D:22:TRP:CE3	1:D:23:SER:N	2.61	0.68
1:A:101:VAL:HG13	1:A:120:THR:HG23	1.74	0.68
1:C:111:ARG:CZ	1:C:117:ILE:HD12	2.23	0.68
1:B:106:ASP:O	1:B:116:GLU:HB3	1.94	0.68
1:B:100:PHE:N	1:B:123:ILE:HD11	2.09	0.68
1:B:100:PHE:N	1:B:123:ILE:CD1	2.53	0.68
1:C:79:SER:O	1:C:82:VAL:HG23	1.93	0.68
1:A:119:VAL:CG2	1:A:143:LEU:HB3	2.24	0.67
1:B:136:VAL:CG2	1:B:137:LYS:H	2.07	0.67
1:C:102:ILE:HG13	1:C:103:GLY:N	2.07	0.67
1:D:130:THR:C	1:D:132:ASP:H	2.02	0.67
1:C:141:ARG:O	1:C:145:LYS:HG3	1.94	0.67
1:D:159:VAL:HG12	1:D:160:PHE:N	2.10	0.67
1:C:108:VAL:O	1:C:115:LEU:HD13	1.94	0.67
1:A:19:VAL:HG23	1:A:19:VAL:O	1.94	0.66
1:A:37:LEU:HB2	1:A:51:LEU:HD11	1.76	0.66
1:B:87:LEU:HD11	1:B:89:PHE:HD2	1.59	0.66
1:A:86:TYR:N	1:A:140:LEU:HD23	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:O	1:B:142:ASP:N	2.29	0.66
1:B:170:VAL:CG1	1:B:171:TRP:N	2.57	0.66
1:C:69:THR:HA	1:C:157:CYS:CB	2.23	0.66
1:C:30:LEU:HD12	1:C:31:GLU:H	1.59	0.66
1:D:91:ILE:HG12	1:D:170:VAL:CG2	2.26	0.66
1:C:8:LEU:HD12	1:C:9:LEU:HD23	1.77	0.66
1:D:113:TYR:HD2	1:D:113:TYR:N	1.91	0.66
1:D:170:VAL:HG22	1:D:171:TRP:N	2.10	0.66
1:A:89:PHE:HD1	1:A:91:ILE:HD11	1.46	0.65
1:A:86:TYR:CE2	1:A:137:LYS:HD3	2.30	0.65
1:D:53:LEU:HB3	1:D:170:VAL:HG13	1.77	0.65
1:A:37:LEU:HD13	1:A:37:LEU:N	2.11	0.65
1:A:40:ASP:HB2	1:A:52:ARG:NH1	2.11	0.65
1:A:151:ASP:C	1:A:153:SER:H	2.05	0.65
1:B:50:THR:HB	1:B:172:PHE:O	1.97	0.65
1:C:101:VAL:HG23	1:C:161:SER:O	1.96	0.65
1:A:140:LEU:HD21	1:A:177:ILE:CG2	2.26	0.65
1:C:55:VAL:HG22	1:C:55:VAL:O	1.95	0.65
1:A:140:LEU:HD11	1:A:144:MET:HE3	1.78	0.65
1:D:59:VAL:HG23	1:D:62:GLY:N	2.11	0.65
1:B:99:ASP:OD1	1:B:123:ILE:CD1	2.45	0.64
1:D:158:LEU:HD22	1:D:159:VAL:N	2.12	0.64
1:D:170:VAL:CG2	1:D:171:TRP:N	2.59	0.64
1:C:31:GLU:OE1	1:C:52:ARG:NH1	2.30	0.64
1:C:130:THR:C	1:C:132:ASP:N	2.54	0.64
1:A:100:PHE:O	1:A:123:ILE:HD13	1.98	0.64
1:B:53:LEU:HD23	1:B:172:PHE:HE1	1.62	0.64
1:A:123:ILE:O	1:A:124:SER:C	2.40	0.64
1:C:67:LEU:HD21	1:C:105:ARG:NH1	2.11	0.64
1:C:101:VAL:HG13	1:C:122:VAL:HG13	1.80	0.64
1:D:10:ASP:OD2	1:D:178:THR:CG2	2.40	0.64
1:D:158:LEU:HD22	1:D:159:VAL:H	1.61	0.64
1:B:33:ILE:O	1:B:34:GLY:C	2.40	0.64
1:B:87:LEU:HD11	1:B:89:PHE:CD2	2.33	0.64
1:A:100:PHE:HA	1:A:163:ARG:HB3	1.79	0.64
1:D:99:ASP:OD1	1:D:124:SER:OG	2.15	0.64
1:B:102:ILE:HA	1:B:159:VAL:O	1.97	0.64
1:C:48:LEU:N	1:C:48:LEU:HD23	2.12	0.64
1:B:87:LEU:HD12	1:B:87:LEU:C	2.22	0.63
1:C:78:LEU:O	1:C:80:GLN:N	2.31	0.63
1:D:148:ASN:C	1:D:148:ASN:OD1	2.39	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:C	1:A:145:LYS:N	2.56	0.63
1:A:51:LEU:HD12	1:A:52:ARG:N	2.14	0.63
1:C:87:LEU:HD12	1:C:104:PHE:CZ	2.34	0.63
1:A:71:ARG:O	1:A:72:GLY:C	2.39	0.63
1:D:106:ASP:HB2	1:D:154:SER:O	1.99	0.63
1:C:22:TRP:O	1:C:67:LEU:HD12	1.98	0.63
1:D:179:SER:OG	1:D:180:GLU:N	2.30	0.63
1:B:20:VAL:O	1:B:69:THR:HG23	1.99	0.63
1:C:126:TYR:N	1:C:126:TYR:CD2	2.63	0.63
1:B:8:LEU:HG	1:B:9:LEU:N	2.12	0.63
1:C:111:ARG:NE	1:C:117:ILE:HD12	2.13	0.63
1:D:48:LEU:N	1:D:48:LEU:HD22	2.14	0.62
1:A:130:THR:C	1:A:132:ASP:N	2.57	0.62
1:D:140:LEU:O	1:D:141:ARG:C	2.41	0.62
1:A:6:ARG:CG	1:A:8:LEU:HD21	2.25	0.62
1:A:54:ASN:HD22	1:A:55:VAL:H	1.45	0.62
1:A:64:TRP:CD1	1:A:162:LYS:HB2	2.35	0.62
1:D:99:ASP:CA	1:D:123:ILE:HD11	2.30	0.62
1:B:71:ARG:O	1:B:72:GLY:C	2.42	0.62
1:B:54:ASN:ND2	1:B:55:VAL:N	2.47	0.62
1:B:82:VAL:HG12	1:B:83:GLU:H	1.61	0.62
1:B:130:THR:C	1:B:132:ASP:N	2.58	0.62
1:C:172:PHE:HB3	1:C:175:ILE:HD11	1.81	0.62
1:B:146:ILE:C	1:B:148:ASN:H	2.05	0.61
1:A:88:GLU:C	1:A:89:PHE:CD2	2.79	0.61
1:D:53:LEU:C	1:D:53:LEU:HD12	2.24	0.61
1:D:123:ILE:HG12	1:D:124:SER:N	2.15	0.61
1:B:13:ILE:HG22	1:B:175:ILE:HB	1.81	0.61
1:C:20:VAL:O	1:C:69:THR:CG2	2.45	0.61
1:A:26:GLY:HA3	1:A:61:SER:OG	2.00	0.61
1:B:41:THR:C	1:B:43:VAL:H	2.07	0.61
1:B:100:PHE:H	1:B:123:ILE:HD13	1.61	0.61
1:C:54:ASN:CA	1:C:169:THR:CG2	2.74	0.61
1:D:54:ASN:HD22	1:D:55:VAL:N	1.98	0.61
1:D:91:ILE:HD11	1:D:129:VAL:HG13	1.80	0.61
1:A:140:LEU:HD12	1:A:144:MET:CE	2.24	0.61
1:C:103:GLY:O	1:C:158:LEU:HD12	2.00	0.61
1:B:57:THR:HG22	1:B:58:THR:H	1.66	0.61
1:C:59:VAL:CG1	1:C:162:LYS:HD2	2.28	0.61
1:C:65:ILE:HG13	1:C:66:SER:N	2.14	0.61
1:C:88:GLU:OE2	1:C:135:HIS:CE1	2.53	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ARG:HE	1:C:117:ILE:CD1	2.14	0.60
1:D:55:VAL:HG22	1:D:55:VAL:O	2.00	0.60
1:B:125:ASN:N	1:B:125:ASN:ND2	2.49	0.60
1:A:33:ILE:O	1:A:33:ILE:CG2	2.48	0.60
1:A:57:THR:OG1	1:B:34:GLY:N	2.35	0.60
1:B:104:PHE:HE1	1:B:158:LEU:HB2	1.67	0.60
1:D:16:ASP:HB3	1:D:48:LEU:HD12	1.83	0.60
1:C:59:VAL:HG11	1:C:162:LYS:CD	2.28	0.60
1:A:151:ASP:O	1:A:153:SER:N	2.35	0.60
1:C:101:VAL:CG1	1:C:122:VAL:HG13	2.31	0.60
1:C:108:VAL:CG1	1:C:111:ARG:HB3	2.31	0.60
1:D:92:LYS:O	1:D:170:VAL:HG23	2.01	0.60
1:A:148:ASN:OD1	1:A:148:ASN:C	2.45	0.60
1:B:179:SER:OG	1:B:180:GLU:N	2.35	0.60
1:B:139:PRO:HG2	1:B:142:ASP:OD2	2.01	0.59
1:C:143:LEU:C	1:C:145:LYS:H	2.09	0.59
1:B:65:ILE:HD12	1:B:66:SER:N	2.18	0.59
1:B:133:TRP:HA	1:B:133:TRP:CE3	2.36	0.59
1:C:119:VAL:HG22	1:C:150:PHE:CD1	2.37	0.59
1:A:78:LEU:O	1:A:80:GLN:N	2.34	0.59
1:B:8:LEU:HG	1:B:9:LEU:H	1.65	0.59
1:D:82:VAL:HG12	1:D:83:GLU:H	1.67	0.59
1:C:92:LYS:HD3	1:C:133:TRP:HE1	1.63	0.59
1:C:102:ILE:HD12	1:C:160:PHE:CE2	2.34	0.59
1:D:148:ASN:OD1	1:D:149:GLY:N	2.36	0.59
1:D:51:LEU:HB3	1:D:172:PHE:HB2	1.84	0.59
1:D:53:LEU:HG	1:D:53:LEU:O	2.03	0.59
1:A:67:LEU:C	1:A:68:LEU:HD13	2.28	0.59
1:A:127:VAL:CG1	1:A:128:THR:O	2.44	0.59
1:C:108:VAL:HG12	1:C:111:ARG:HB3	1.84	0.59
1:C:164:TYR:HB3	1:C:166:ASP:OD2	2.03	0.59
1:D:87:LEU:H	1:D:140:LEU:CD2	2.15	0.59
1:D:95:GLU:O	1:D:95:GLU:CG	2.51	0.59
1:D:104:PHE:N	1:D:104:PHE:CD2	2.71	0.59
1:B:169:THR:HG22	1:B:170:VAL:H	1.66	0.58
1:C:8:LEU:HG	1:C:9:LEU:H	1.67	0.58
1:C:151:ASP:C	1:C:151:ASP:OD1	2.46	0.58
1:A:13:ILE:HG12	1:A:70:LEU:CD2	2.33	0.58
1:A:88:GLU:OE1	1:A:135:HIS:HE1	1.78	0.58
1:B:104:PHE:CE1	1:B:158:LEU:HB2	2.37	0.58
1:B:125:ASN:C	1:D:20:VAL:HG11	2.27	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:PHE:N	1:D:89:PHE:CD2	2.70	0.58
1:D:126:TYR:CD1	1:D:138:ILE:HG13	2.38	0.58
1:A:174:ASP:C	1:A:175:ILE:HD12	2.27	0.58
1:B:31:GLU:CD	1:B:52:ARG:HH11	2.10	0.58
1:C:8:LEU:CG	1:C:9:LEU:N	2.62	0.58
1:C:110:GLU:OE1	1:C:110:GLU:N	2.33	0.58
1:A:159:VAL:C	1:A:160:PHE:CD1	2.82	0.58
1:C:141:ARG:O	1:C:145:LYS:CG	2.52	0.58
1:D:87:LEU:HD12	1:D:176:LYS:O	2.04	0.58
1:C:78:LEU:HG	1:C:155:VAL:HG21	1.85	0.58
1:C:176:LYS:HG3	1:C:178:THR:HG23	1.85	0.58
1:D:33:ILE:O	1:D:34:GLY:C	2.47	0.58
1:D:138:ILE:HG22	1:D:139:PRO:O	2.04	0.58
1:D:169:THR:CG2	1:D:170:VAL:H	2.15	0.58
1:D:48:LEU:N	1:D:48:LEU:CD2	2.67	0.58
1:A:59:VAL:HG12	1:A:62:GLY:H	1.69	0.58
1:B:103:GLY:HA3	1:B:119:VAL:O	2.04	0.57
1:B:39:VAL:HG22	1:B:39:VAL:O	2.02	0.57
1:A:127:VAL:HG21	1:A:136:VAL:HG11	1.85	0.57
1:B:53:LEU:HD23	1:B:172:PHE:CE1	2.38	0.57
1:C:87:LEU:H	1:C:140:LEU:CD2	2.17	0.57
1:D:88:GLU:C	1:D:89:PHE:HD2	2.12	0.57
1:D:91:ILE:HA	1:D:133:TRP:HZ3	1.68	0.57
1:D:22:TRP:CZ3	1:D:24:GLY:HA3	2.39	0.57
1:D:143:LEU:C	1:D:145:LYS:H	2.13	0.57
1:A:68:LEU:O	1:A:157:CYS:HB2	2.05	0.57
1:D:36:THR:HG23	1:D:37:LEU:N	2.20	0.57
1:D:11:VAL:HG23	1:D:177:ILE:HB	1.86	0.57
1:D:45:TYR:O	1:D:46:ASN:CB	2.47	0.57
1:A:50:THR:CG2	1:A:172:PHE:O	2.38	0.57
1:B:91:ILE:HA	1:B:133:TRP:HZ3	1.68	0.57
1:D:102:ILE:HG22	1:D:121:THR:O	2.05	0.57
1:D:100:PHE:H	1:D:123:ILE:HD13	1.67	0.56
1:D:170:VAL:CG2	1:D:171:TRP:H	2.18	0.56
1:A:22:TRP:CE3	1:A:23:SER:N	2.73	0.56
1:C:8:LEU:CD1	1:C:9:LEU:H	2.18	0.56
1:D:169:THR:HG21	1:D:171:TRP:CZ2	2.40	0.56
1:B:99:ASP:HA	1:B:123:ILE:HD11	1.87	0.56
1:B:123:ILE:HD13	1:B:123:ILE:H	1.70	0.56
1:B:156:THR:HG23	1:B:157:CYS:SG	2.45	0.56
1:C:67:LEU:HD12	1:C:67:LEU:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:PHE:HB3	1:D:175:ILE:HA	1.87	0.56
1:D:130:THR:C	1:D:132:ASP:N	2.63	0.56
1:D:156:THR:OG1	1:D:157:CYS:N	2.38	0.56
1:D:12:GLN:NE2	1:D:14:PHE:O	2.39	0.56
1:A:89:PHE:HE1	1:A:91:ILE:CD1	2.14	0.56
1:D:151:ASP:O	1:D:154:SER:HB2	2.06	0.56
1:A:14:PHE:CD2	1:A:51:LEU:HD23	2.40	0.56
1:A:15:LYS:HG2	1:A:48:LEU:HD22	1.86	0.56
1:A:33:ILE:O	1:A:33:ILE:HG22	2.05	0.56
1:A:56:GLN:HB3	1:B:33:ILE:HD12	1.87	0.56
1:A:23:SER:CB	1:A:37:LEU:CD1	2.83	0.56
1:A:104:PHE:HB2	1:A:119:VAL:HG12	1.88	0.56
1:C:86:TYR:HA	1:C:138:ILE:O	2.06	0.56
1:A:146:ILE:C	1:A:148:ASN:H	2.09	0.56
1:B:124:SER:OG	1:B:125:ASN:ND2	2.39	0.56
1:C:51:LEU:HB3	1:C:172:PHE:HB2	1.88	0.56
1:A:72:GLY:O	1:A:73:TRP:HB2	2.07	0.55
1:C:8:LEU:HB3	1:C:180:GLU:HG2	1.87	0.55
1:D:121:THR:HG23	1:D:122:VAL:N	2.21	0.55
1:A:22:TRP:CZ3	1:A:24:GLY:CA	2.89	0.55
1:D:106:ASP:C	1:D:106:ASP:OD1	2.47	0.55
1:D:106:ASP:O	1:D:116:GLU:HB3	2.07	0.55
1:D:131:THR:O	1:D:131:THR:CG2	2.54	0.55
1:A:98:GLU:H	1:A:129:VAL:HG21	1.71	0.55
1:B:156:THR:CG2	1:B:157:CYS:N	2.68	0.55
1:D:113:TYR:N	1:D:113:TYR:CD2	2.62	0.55
1:A:151:ASP:O	1:A:154:SER:N	2.38	0.55
1:A:87:LEU:HD12	1:A:88:GLU:N	2.22	0.55
1:C:8:LEU:HD12	1:C:9:LEU:H	1.72	0.55
1:B:8:LEU:O	1:B:8:LEU:HD23	2.07	0.55
1:C:54:ASN:HD22	1:C:169:THR:CG2	2.20	0.55
1:D:59:VAL:HG23	1:D:62:GLY:CA	2.37	0.55
1:A:101:VAL:HG11	1:A:120:THR:CG2	2.36	0.55
1:A:127:VAL:CG2	1:A:136:VAL:HG11	2.36	0.55
1:A:133:TRP:HA	1:A:133:TRP:CE3	2.41	0.55
1:A:159:VAL:C	1:A:160:PHE:HD1	2.15	0.55
1:B:31:GLU:CD	1:B:52:ARG:NH1	2.66	0.55
1:B:57:THR:CG2	1:B:58:THR:H	2.19	0.55
1:B:117:ILE:CG2	1:B:118:ASP:N	2.68	0.55
1:D:151:ASP:C	1:D:153:SER:H	2.15	0.54
1:A:158:LEU:C	1:A:159:VAL:HG23	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD23	1:B:8:LEU:C	2.32	0.54
1:A:88:GLU:C	1:A:89:PHE:HD2	2.15	0.54
1:A:102:ILE:HG22	1:A:121:THR:HG23	1.90	0.54
1:A:151:ASP:C	1:A:151:ASP:OD1	2.50	0.54
1:A:23:SER:OG	1:A:37:LEU:HD11	2.07	0.54
1:C:23:SER:HA	1:C:65:ILE:O	2.07	0.54
1:C:88:GLU:OE2	1:C:135:HIS:HE1	1.89	0.54
1:C:111:ARG:HE	1:C:117:ILE:HD12	1.72	0.54
1:D:87:LEU:HG	1:D:88:GLU:N	2.16	0.54
1:A:140:LEU:O	1:A:141:ARG:C	2.51	0.54
1:D:72:GLY:O	1:D:73:TRP:HB2	2.06	0.54
1:A:78:LEU:O	1:A:81:TYR:HD1	1.90	0.54
1:B:102:ILE:HG21	1:B:123:ILE:HG22	1.89	0.54
1:C:47:GLY:C	1:C:48:LEU:HD23	2.32	0.54
1:D:117:ILE:HG22	1:D:118:ASP:N	2.23	0.54
1:B:158:LEU:HG	1:B:159:VAL:N	2.21	0.54
1:C:68:LEU:HD23	1:C:68:LEU:N	1.98	0.54
1:D:78:LEU:O	1:D:80:GLN:N	2.40	0.54
1:D:92:LYS:HB3	1:D:133:TRP:CD2	2.42	0.54
1:C:8:LEU:CG	1:C:9:LEU:H	2.21	0.54
1:C:37:LEU:HD23	1:C:68:LEU:HD11	1.89	0.54
1:A:89:PHE:HB3	1:A:175:ILE:HG13	1.89	0.54
1:A:101:VAL:HG12	1:A:102:ILE:H	1.73	0.54
1:C:19:VAL:O	1:C:36:THR:HG21	2.07	0.54
1:B:20:VAL:HG23	1:B:69:THR:OG1	2.09	0.53
1:B:22:TRP:HB3	1:B:67:LEU:HD12	1.90	0.53
1:C:122:VAL:HG11	1:C:163:ARG:HD3	1.90	0.53
1:D:112:VAL:HG23	1:D:113:TYR:N	2.24	0.53
1:A:22:TRP:CZ3	1:A:24:GLY:HA3	2.44	0.53
1:A:101:VAL:CG1	1:A:102:ILE:N	2.71	0.53
1:A:117:ILE:HG22	1:A:118:ASP:H	1.73	0.53
1:A:170:VAL:C	1:A:171:TRP:CE3	2.87	0.53
1:D:103:GLY:O	1:D:159:VAL:N	2.41	0.53
1:B:136:VAL:HG23	1:B:137:LYS:H	1.73	0.53
1:A:127:VAL:HG12	1:A:128:THR:N	2.24	0.53
1:B:8:LEU:CD2	1:B:179:SER:HB3	2.39	0.53
1:D:65:ILE:HG13	1:D:66:SER:N	2.22	0.53
1:D:66:SER:HB3	1:D:160:PHE:HB2	1.90	0.53
1:A:117:ILE:HG22	1:A:118:ASP:N	2.23	0.53
1:B:66:SER:O	1:B:159:VAL:HA	2.08	0.53
1:C:105:ARG:HA	1:C:117:ILE:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:THR:HG21	1:A:171:TRP:HB3	1.91	0.53
1:B:71:ARG:O	1:B:74:ASN:HB2	2.08	0.53
1:C:101:VAL:HG13	1:C:122:VAL:CG1	2.38	0.53
1:A:70:LEU:HG	1:A:157:CYS:HA	1.91	0.53
1:B:31:GLU:OE1	1:B:52:ARG:NH1	2.33	0.53
1:A:48:LEU:HB3	1:A:49:PRO:HD2	1.90	0.53
1:B:116:GLU:C	1:B:117:ILE:HD12	2.34	0.53
1:A:19:VAL:HG23	1:A:36:THR:OG1	2.08	0.52
1:A:78:LEU:O	1:A:81:TYR:N	2.36	0.52
1:B:46:ASN:CG	1:B:46:ASN:O	2.53	0.52
1:C:89:PHE:HE1	1:C:91:ILE:HG21	1.74	0.52
1:A:13:ILE:HG12	1:A:70:LEU:HD22	1.91	0.52
1:A:159:VAL:O	1:A:160:PHE:CD1	2.60	0.52
1:D:67:LEU:HD23	1:D:159:VAL:HG22	1.91	0.52
1:D:111:ARG:CG	1:D:113:TYR:HE2	2.22	0.52
1:D:8:LEU:CD1	1:D:9:LEU:H	2.05	0.52
1:D:87:LEU:N	1:D:140:LEU:CD2	2.72	0.52
1:B:117:ILE:HG22	1:B:118:ASP:N	2.24	0.52
1:A:45:TYR:O	1:A:46:ASN:OD1	2.27	0.52
1:C:140:LEU:O	1:C:142:ASP:N	2.43	0.52
1:D:163:ARG:HD3	1:D:164:TYR:CZ	2.45	0.52
1:A:142:ASP:OD2	1:A:142:ASP:N	2.41	0.52
1:B:168:PHE:CD1	1:B:168:PHE:C	2.88	0.52
1:A:131:THR:O	1:A:131:THR:HG22	2.10	0.52
1:C:78:LEU:O	1:C:79:SER:C	2.53	0.52
1:D:109:TYR:N	1:D:110:GLU:OE1	2.42	0.52
1:D:168:PHE:C	1:D:168:PHE:CD1	2.88	0.51
1:D:29:GLU:HG2	1:D:59:VAL:HG12	1.93	0.51
1:D:64:TRP:CZ2	1:D:162:LYS:HA	2.45	0.51
1:D:91:ILE:C	1:D:91:ILE:CD1	2.77	0.51
1:C:124:SER:HA	1:C:127:VAL:O	2.10	0.51
1:D:43:VAL:HG12	1:D:43:VAL:O	2.09	0.51
1:D:126:TYR:N	1:D:126:TYR:CD2	2.78	0.51
1:A:13:ILE:HG21	1:A:158:LEU:HD22	1.93	0.51
1:A:93:GLY:HA2	1:A:170:VAL:HA	1.92	0.51
1:C:146:ILE:O	1:C:148:ASN:CB	2.51	0.51
1:D:130:THR:OG1	1:D:132:ASP:CB	2.56	0.51
1:D:38:PRO:HG2	1:D:52:ARG:HB3	1.93	0.51
1:D:78:LEU:HD12	1:D:155:VAL:HG21	1.91	0.51
1:D:110:GLU:CD	1:D:110:GLU:H	2.19	0.51
1:D:159:VAL:CG1	1:D:160:PHE:N	2.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TYR:O	1:A:127:VAL:HG22	2.10	0.51
1:B:22:TRP:C	1:B:23:SER:OG	2.53	0.51
1:A:162:LYS:HG2	1:A:163:ARG:N	2.25	0.51
1:D:101:VAL:HG23	1:D:161:SER:O	2.10	0.51
1:D:143:LEU:O	1:D:145:LYS:N	2.44	0.51
1:D:150:PHE:O	1:D:152:PRO:HD3	2.11	0.51
1:A:55:VAL:O	1:A:56:GLN:C	2.53	0.50
1:B:54:ASN:HD22	1:B:55:VAL:H	1.59	0.50
1:A:86:TYR:HA	1:A:138:ILE:O	2.11	0.50
1:A:97:GLY:HA2	1:A:129:VAL:HG23	1.93	0.50
1:A:104:PHE:HB2	1:A:119:VAL:CG1	2.42	0.50
1:A:156:THR:OG1	1:A:157:CYS:N	2.44	0.50
1:B:77:ASP:OD1	1:B:153:SER:CB	2.51	0.50
1:C:28:GLY:N	1:C:29:GLU:OE2	2.44	0.50
1:A:14:PHE:C	1:A:14:PHE:HD1	2.17	0.50
1:A:151:ASP:C	1:A:153:SER:N	2.70	0.50
1:C:127:VAL:HG12	1:C:134:GLN:NE2	2.24	0.50
1:B:114:GLY:HA3	1:B:117:ILE:HD11	1.93	0.50
1:C:30:LEU:CD1	1:C:54:ASN:O	2.60	0.50
1:D:105:ARG:HG3	1:D:118:ASP:CG	2.37	0.50
1:A:139:PRO:HB2	1:A:142:ASP:OD2	2.10	0.50
1:D:75:THR:HA	1:D:155:VAL:O	2.11	0.50
1:D:88:GLU:C	1:D:89:PHE:CD2	2.90	0.50
1:D:151:ASP:O	1:D:153:SER:N	2.45	0.50
1:B:91:ILE:CA	1:B:133:TRP:HZ3	2.24	0.50
1:D:130:THR:HG22	1:D:134:GLN:OE1	2.12	0.50
1:D:140:LEU:HD13	1:D:144:MET:CE	2.35	0.50
1:A:23:SER:CB	1:A:37:LEU:HD11	2.42	0.49
1:A:100:PHE:CD1	1:A:100:PHE:C	2.88	0.49
1:B:119:VAL:CG2	1:B:143:LEU:HB3	2.42	0.49
1:D:22:TRP:CZ3	1:D:24:GLY:CA	2.95	0.49
1:A:48:LEU:CB	1:A:49:PRO:HD2	2.42	0.49
1:A:51:LEU:HD12	1:A:51:LEU:C	2.37	0.49
1:B:13:ILE:HG22	1:B:14:PHE:H	1.76	0.49
1:D:66:SER:CB	1:D:160:PHE:HB2	2.42	0.49
1:D:98:GLU:HA	1:D:98:GLU:OE2	2.11	0.49
1:A:97:GLY:CA	1:A:129:VAL:HG23	2.42	0.49
1:D:123:ILE:CG1	1:D:124:SER:N	2.76	0.49
1:A:6:ARG:HB3	1:A:8:LEU:CD2	2.43	0.49
1:C:19:VAL:HG13	1:C:20:VAL:N	2.27	0.49
1:A:15:LYS:CE	1:A:48:LEU:HD21	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASN:O	1:A:46:ASN:CG	2.55	0.49
1:B:29:GLU:OE1	1:B:59:VAL:HB	2.13	0.49
1:D:67:LEU:HB3	1:D:157:CYS:SG	2.52	0.49
1:B:112:VAL:C	1:B:114:GLY:H	2.20	0.49
1:D:31:GLU:O	1:D:38:PRO:HD3	2.12	0.49
1:B:37:LEU:CD1	1:B:37:LEU:N	2.75	0.49
1:C:119:VAL:HG13	1:C:150:PHE:CD1	2.48	0.49
1:D:59:VAL:HG23	1:D:62:GLY:HA2	1.95	0.48
1:A:37:LEU:N	1:A:37:LEU:CD1	2.76	0.48
1:A:108:VAL:O	1:A:115:LEU:HD13	2.14	0.48
1:C:111:ARG:HH21	1:C:117:ILE:CD1	2.23	0.48
1:C:143:LEU:C	1:C:145:LYS:N	2.71	0.48
1:D:12:GLN:HG2	1:D:15:LYS:HB2	1.96	0.48
1:D:119:VAL:HG12	1:D:148:ASN:HD21	1.79	0.48
1:A:67:LEU:O	1:A:68:LEU:CD1	2.62	0.48
1:D:99:ASP:OD2	1:D:122:VAL:HG12	2.13	0.48
1:C:170:VAL:C	1:C:171:TRP:CE3	2.92	0.48
1:A:6:ARG:HB3	1:A:7:LYS:H	1.40	0.48
1:A:98:GLU:H	1:A:129:VAL:CG2	2.27	0.48
1:A:94:LYS:N	1:A:98:GLU:OE1	2.46	0.48
1:A:158:LEU:C	1:A:159:VAL:CG2	2.83	0.48
1:C:30:LEU:HD12	1:C:54:ASN:O	2.14	0.48
1:B:91:ILE:CA	1:B:133:TRP:CZ3	2.97	0.48
1:C:67:LEU:CD2	1:C:105:ARG:NH1	2.76	0.48
1:D:85:GLY:O	1:D:139:PRO:HA	2.13	0.48
1:A:135:HIS:ND1	1:A:136:VAL:N	2.61	0.47
1:A:119:VAL:HG22	1:A:143:LEU:HD23	1.96	0.47
1:B:41:THR:C	1:B:43:VAL:N	2.69	0.47
1:B:63:TRP:HZ3	1:B:65:ILE:HG22	1.78	0.47
1:B:170:VAL:C	1:B:171:TRP:CE3	2.92	0.47
1:D:111:ARG:NH2	1:D:117:ILE:CG1	2.70	0.47
1:A:102:ILE:CG2	1:A:121:THR:HG23	2.44	0.47
1:B:140:LEU:CD1	1:B:144:MET:HE3	2.45	0.47
1:A:6:ARG:HB3	1:A:8:LEU:HD22	1.97	0.47
1:B:130:THR:HB	1:B:132:ASP:HB2	1.95	0.47
1:C:50:THR:HG21	1:C:171:TRP:HB3	1.96	0.47
1:C:51:LEU:HD12	1:C:51:LEU:HA	1.47	0.47
1:B:106:ASP:OD1	1:B:117:ILE:N	2.37	0.47
1:B:169:THR:CG2	1:B:170:VAL:N	2.74	0.47
1:C:39:VAL:CG1	1:C:39:VAL:O	2.63	0.47
1:D:140:LEU:HB3	1:D:144:MET:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:THR:O	1:D:157:CYS:HB3	2.15	0.47
1:C:87:LEU:CD1	1:C:104:PHE:CZ	2.97	0.47
1:A:173:SER:C	1:A:175:ILE:HD12	2.39	0.47
1:B:68:LEU:HD12	1:B:158:LEU:HD23	1.96	0.47
1:C:124:SER:OG	1:C:125:ASN:N	2.44	0.47
1:D:9:LEU:O	1:D:81:TYR:OH	2.18	0.47
1:D:57:THR:HB	1:D:58:THR:H	1.43	0.47
1:D:168:PHE:HD1	1:D:169:THR:CA	2.28	0.47
1:B:37:LEU:HA	1:B:38:PRO:HD3	1.67	0.46
1:B:162:LYS:HD2	1:B:165:ALA:HA	1.96	0.46
1:C:36:THR:HG23	1:C:37:LEU:N	2.30	0.46
1:A:7:LYS:H	1:A:8:LEU:HD22	1.79	0.46
1:D:103:GLY:C	1:D:104:PHE:CD2	2.93	0.46
1:A:168:PHE:HD1	1:A:169:THR:O	1.98	0.46
1:B:179:SER:O	1:B:180:GLU:HB3	2.16	0.46
1:A:56:GLN:HB3	1:B:33:ILE:CD1	2.45	0.46
1:A:66:SER:O	1:A:159:VAL:HA	2.14	0.46
1:A:51:LEU:HB3	1:A:172:PHE:HB2	1.96	0.46
1:B:144:MET:SD	1:B:152:PRO:HB3	2.55	0.46
1:C:78:LEU:HD12	1:C:144:MET:HE1	1.98	0.46
1:C:151:ASP:O	1:C:153:SER:N	2.49	0.46
1:D:33:ILE:C	1:D:35:ASP:N	2.70	0.46
1:C:102:ILE:HA	1:C:159:VAL:O	2.16	0.46
1:A:158:LEU:HG	1:A:159:VAL:N	2.31	0.46
1:D:54:ASN:HD22	1:D:54:ASN:C	2.24	0.46
1:D:147:ASN:OD1	1:D:147:ASN:N	2.49	0.46
1:A:113:TYR:O	1:A:113:TYR:CD1	2.69	0.46
1:A:121:THR:OG1	1:A:122:VAL:N	2.49	0.46
1:C:54:ASN:HD22	1:C:169:THR:HG23	1.80	0.46
1:C:138:ILE:HA	1:C:139:PRO:HD2	1.38	0.46
1:A:126:TYR:N	1:A:126:TYR:CD2	2.84	0.46
1:A:36:THR:HG23	1:A:37:LEU:O	2.16	0.45
1:A:39:VAL:HG13	1:A:39:VAL:O	2.16	0.45
1:B:23:SER:HB3	1:B:66:SER:OG	2.15	0.45
1:C:66:SER:O	1:C:159:VAL:HA	2.17	0.45
1:D:99:ASP:C	1:D:123:ILE:HD11	2.40	0.45
1:D:100:PHE:N	1:D:123:ILE:CD1	2.60	0.45
1:C:111:ARG:HG2	1:C:114:GLY:O	2.13	0.45
1:C:121:THR:HG21	1:C:126:TYR:HE2	1.81	0.45
1:D:22:TRP:CZ3	1:D:24:GLY:N	2.84	0.45
1:A:23:SER:OG	1:A:37:LEU:CD1	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:CD1	1:A:52:ARG:N	2.77	0.45
1:B:156:THR:HG23	1:B:157:CYS:N	2.30	0.45
1:C:22:TRP:HA	1:C:35:ASP:O	2.16	0.45
1:C:111:ARG:HE	1:C:117:ILE:HD11	1.81	0.45
1:D:33:ILE:HA	1:D:33:ILE:HD12	1.27	0.45
1:B:91:ILE:HA	1:B:133:TRP:CZ3	2.50	0.45
1:C:148:ASN:O	1:C:148:ASN:ND2	2.49	0.45
1:A:67:LEU:O	1:A:68:LEU:HD13	2.17	0.45
1:A:100:PHE:O	1:A:123:ILE:HD11	2.16	0.45
1:A:139:PRO:HG2	1:A:142:ASP:OD1	2.17	0.45
1:B:8:LEU:HD22	1:B:179:SER:HB3	1.98	0.45
1:B:27:MET:HE3	1:B:27:MET:HB2	1.57	0.45
1:B:78:LEU:HD12	1:B:155:VAL:HG21	1.99	0.45
1:B:151:ASP:O	1:B:153:SER:N	2.50	0.45
1:C:59:VAL:HG22	1:C:62:GLY:H	1.82	0.45
1:C:175:ILE:H	1:C:175:ILE:HG12	1.44	0.45
1:C:100:PHE:H	1:C:123:ILE:CD1	2.30	0.45
1:C:119:VAL:CG2	1:C:150:PHE:CE1	2.94	0.45
1:C:143:LEU:O	1:C:145:LYS:N	2.27	0.45
1:D:98:GLU:O	1:D:129:VAL:HG21	2.17	0.45
1:C:119:VAL:HG13	1:C:150:PHE:HD1	1.80	0.45
1:C:122:VAL:CG1	1:C:163:ARG:HD3	2.47	0.45
1:A:98:GLU:N	1:A:129:VAL:HG21	2.32	0.45
1:B:22:TRP:HA	1:B:35:ASP:O	2.17	0.45
1:A:14:PHE:CD2	1:A:51:LEU:CD2	2.99	0.44
1:A:66:SER:N	1:A:160:PHE:O	2.37	0.44
1:A:80:GLN:HE21	1:A:80:GLN:HB3	1.63	0.44
1:A:130:THR:O	1:A:132:ASP:N	2.47	0.44
1:D:71:ARG:O	1:D:74:ASN:HB2	2.17	0.44
1:A:106:ASP:C	1:A:106:ASP:OD2	2.58	0.44
1:B:13:ILE:CG2	1:B:175:ILE:HB	2.45	0.44
1:D:155:VAL:H	1:D:155:VAL:HG23	1.51	0.44
1:A:14:PHE:CD1	1:A:15:LYS:N	2.86	0.44
1:B:87:LEU:CD1	1:B:89:PHE:HD2	2.26	0.44
1:D:48:LEU:HA	1:D:49:PRO:HD2	1.40	0.44
1:B:23:SER:OG	1:B:36:THR:HA	2.17	0.44
1:B:70:LEU:HD12	1:B:157:CYS:HA	2.00	0.44
1:C:125:ASN:N	1:C:125:ASN:HD22	2.14	0.44
1:D:106:ASP:OD1	1:D:107:LYS:N	2.50	0.44
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.51	0.44
1:A:68:LEU:O	1:A:157:CYS:CB	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HB3	1:C:170:VAL:HG23	1.99	0.44
1:D:19:VAL:O	1:D:36:THR:HG21	2.18	0.44
1:A:89:PHE:CD2	1:A:89:PHE:N	2.86	0.44
1:B:41:THR:O	1:B:43:VAL:N	2.51	0.44
1:D:31:GLU:HB2	1:D:56:GLN:CD	2.43	0.44
1:B:40:ASP:OD2	1:B:41:THR:N	2.50	0.44
1:C:40:ASP:OD2	1:C:40:ASP:C	2.59	0.44
1:C:53:LEU:HB3	1:C:170:VAL:CG2	2.48	0.44
1:C:102:ILE:HG22	1:C:121:THR:O	2.18	0.44
1:D:179:SER:C	1:D:180:GLU:HG3	2.42	0.44
1:D:163:ARG:HD3	1:D:164:TYR:CD2	2.53	0.44
1:B:149:GLY:O	1:B:150:PHE:C	2.61	0.43
1:A:35:ASP:OD1	1:A:35:ASP:N	2.51	0.43
1:A:37:LEU:HD13	1:A:37:LEU:H	1.83	0.43
1:B:20:VAL:H	1:B:20:VAL:HG22	1.41	0.43
1:B:57:THR:HG22	1:B:58:THR:HG22	1.99	0.43
1:B:151:ASP:C	1:B:153:SER:H	2.26	0.43
1:A:136:VAL:CG2	1:A:137:LYS:N	2.80	0.43
1:D:51:LEU:HD12	1:D:51:LEU:HA	1.84	0.43
1:A:63:TRP:HZ3	1:A:65:ILE:HG22	1.83	0.43
1:A:104:PHE:O	1:A:118:ASP:HA	2.19	0.43
1:A:127:VAL:HG12	1:A:128:THR:C	2.39	0.43
1:B:92:LYS:HB2	1:B:133:TRP:CZ3	2.54	0.43
1:C:67:LEU:HD12	1:C:67:LEU:N	2.33	0.43
1:C:151:ASP:C	1:C:153:SER:H	2.25	0.43
1:D:98:GLU:CD	1:D:168:PHE:HB3	2.37	0.43
1:D:91:ILE:CG1	1:D:170:VAL:CG2	2.97	0.43
1:B:22:TRP:CE3	1:B:23:SER:N	2.87	0.43
1:D:170:VAL:HG23	1:D:171:TRP:H	1.84	0.43
1:A:51:LEU:C	1:A:51:LEU:CD1	2.92	0.43
1:A:87:LEU:HD13	1:A:177:ILE:HD13	2.01	0.43
1:B:132:ASP:C	1:B:133:TRP:O	2.61	0.43
1:A:111:ARG:NH2	1:A:117:ILE:HG13	2.33	0.43
1:A:115:LEU:HD13	1:A:115:LEU:HA	1.83	0.43
1:A:113:TYR:CD1	1:A:113:TYR:C	2.97	0.43
1:B:115:LEU:HD13	1:B:115:LEU:HA	1.68	0.43
1:C:19:VAL:HG13	1:C:20:VAL:O	2.17	0.43
1:C:116:GLU:C	1:C:117:ILE:HG13	2.43	0.43
1:B:67:LEU:HA	1:B:158:LEU:O	2.19	0.42
1:A:19:VAL:HG23	1:A:36:THR:HG1	1.84	0.42
1:A:126:TYR:C	1:A:127:VAL:CG2	2.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:C	1:B:145:LYS:N	2.61	0.42
1:C:86:TYR:HA	1:C:140:LEU:HD23	2.01	0.42
1:D:36:THR:HG23	1:D:37:LEU:O	2.19	0.42
1:D:151:ASP:HA	1:D:152:PRO:HD3	1.76	0.42
1:A:87:LEU:HD12	1:A:88:GLU:H	1.84	0.42
1:B:34:GLY:O	1:B:35:ASP:HB2	2.18	0.42
1:B:132:ASP:O	1:B:133:TRP:C	2.62	0.42
1:C:89:PHE:CE1	1:C:91:ILE:HG21	2.53	0.42
1:C:127:VAL:CG1	1:C:134:GLN:HE21	2.29	0.42
1:D:22:TRP:HZ3	1:D:65:ILE:HG23	1.84	0.42
1:B:39:VAL:HG23	1:B:40:ASP:N	2.32	0.42
1:C:39:VAL:O	1:C:39:VAL:HG13	2.20	0.42
1:B:78:LEU:O	1:B:81:TYR:N	2.33	0.42
1:C:83:GLU:H	1:C:83:GLU:HG3	1.46	0.42
1:C:33:ILE:C	1:C:35:ASP:H	2.27	0.42
1:A:87:LEU:N	1:A:140:LEU:HD22	2.34	0.42
1:A:101:VAL:CG1	1:A:102:ILE:H	2.33	0.42
1:B:51:LEU:HB3	1:B:172:PHE:HB2	2.02	0.42
1:C:126:TYR:N	1:C:126:TYR:HD2	2.16	0.42
1:D:99:ASP:OD2	1:D:123:ILE:HG12	2.19	0.42
1:A:84:ASN:HD22	1:A:84:ASN:HA	1.73	0.42
1:B:102:ILE:HG13	1:B:160:PHE:CE2	2.55	0.42
1:B:112:VAL:C	1:B:114:GLY:N	2.77	0.42
1:C:121:THR:HG21	1:C:126:TYR:CE2	2.54	0.42
1:A:22:TRP:HA	1:A:35:ASP:O	2.20	0.42
1:A:71:ARG:O	1:A:74:ASN:N	2.46	0.42
1:C:71:ARG:O	1:C:74:ASN:N	2.48	0.42
1:C:104:PHE:O	1:C:118:ASP:HA	2.20	0.42
1:C:175:ILE:HD12	1:C:175:ILE:HG23	1.53	0.42
1:D:58:THR:HA	1:D:167:PRO:HD3	2.02	0.42
1:D:141:ARG:HE	1:D:141:ARG:HB3	1.64	0.42
1:D:173:SER:O	1:D:174:ASP:C	2.62	0.42
1:B:37:LEU:HA	1:B:37:LEU:HD12	1.66	0.41
1:B:98:GLU:OE2	1:B:98:GLU:N	2.53	0.41
1:B:140:LEU:HD11	1:B:144:MET:HE3	2.02	0.41
1:B:151:ASP:C	1:B:151:ASP:OD1	2.63	0.41
1:C:139:PRO:HG3	1:C:142:ASP:OD1	2.20	0.41
1:D:27:MET:HE3	1:D:27:MET:H	1.84	0.41
1:D:105:ARG:HG3	1:D:118:ASP:OD2	2.20	0.41
1:D:138:ILE:HA	1:D:139:PRO:HD2	1.52	0.41
1:C:156:THR:O	1:C:157:CYS:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:VAL:HG13	1:D:83:GLU:CA	2.50	0.41
1:A:12:GLN:OE1	1:A:176:LYS:HD2	2.21	0.41
1:B:54:ASN:ND2	1:B:54:ASN:C	2.78	0.41
1:B:86:TYR:CG	1:B:137:LYS:HD2	2.55	0.41
1:A:163:ARG:HG3	1:A:164:TYR:N	2.35	0.41
1:C:127:VAL:HG11	1:C:134:GLN:HE21	1.82	0.41
1:D:46:ASN:C	1:D:48:LEU:H	2.28	0.41
1:D:91:ILE:CA	1:D:133:TRP:CZ3	2.99	0.41
1:D:117:ILE:HG22	1:D:118:ASP:H	1.83	0.41
1:A:22:TRP:CE3	1:A:23:SER:C	2.98	0.41
1:A:128:THR:O	1:A:134:GLN:NE2	2.53	0.41
1:A:166:ASP:HA	1:A:167:PRO:HD2	1.20	0.41
1:C:99:ASP:OD1	1:C:124:SER:HB3	2.20	0.41
1:A:126:TYR:HE1	1:A:139:PRO:HG2	1.86	0.41
1:C:148:ASN:O	1:C:148:ASN:CG	2.63	0.41
1:D:55:VAL:O	1:D:167:PRO:HB3	2.21	0.41
1:D:103:GLY:HA3	1:D:119:VAL:O	2.20	0.41
1:B:29:GLU:OE2	1:B:63:TRP:O	2.39	0.41
1:C:143:LEU:HD12	1:C:143:LEU:N	2.26	0.41
1:D:143:LEU:C	1:D:145:LYS:N	2.79	0.41
1:A:89:PHE:CG	1:A:175:ILE:HG13	2.55	0.41
1:A:164:TYR:C	1:A:166:ASP:H	2.29	0.41
1:B:103:GLY:O	1:B:158:LEU:HA	2.20	0.41
1:C:12:GLN:OE1	1:C:12:GLN:HA	2.19	0.41
1:C:150:PHE:CD2	1:C:150:PHE:C	2.99	0.41
1:D:72:GLY:O	1:D:73:TRP:CB	2.69	0.41
1:D:130:THR:HG23	1:D:132:ASP:O	2.21	0.41
1:D:151:ASP:C	1:D:151:ASP:OD1	2.64	0.41
1:A:22:TRP:CE3	1:A:23:SER:CA	3.03	0.41
1:B:14:PHE:CG	1:B:15:LYS:N	2.83	0.41
1:B:94:LYS:HB2	1:B:169:THR:HB	2.02	0.41
1:C:48:LEU:HB3	1:C:49:PRO:HD2	2.03	0.41
1:C:106:ASP:CG	1:C:111:ARG:HH22	2.29	0.41
1:D:87:LEU:N	1:D:140:LEU:HD21	2.35	0.41
1:D:91:ILE:CG1	1:D:170:VAL:HG21	2.51	0.41
1:D:104:PHE:HA	1:D:157:CYS:O	2.20	0.41
1:D:177:ILE:HG23	1:D:177:ILE:HD12	1.73	0.41
1:C:90:ASP:C	1:C:91:ILE:HG22	2.45	0.41
1:A:11:VAL:O	1:A:176:LYS:HA	2.21	0.40
1:A:20:VAL:HG21	1:C:18:PRO:CG	2.51	0.40
1:A:81:TYR:N	1:A:81:TYR:CD1	2.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASP:C	1:D:153:SER:N	2.79	0.40
1:B:21:GLY:O	1:B:22:TRP:HB2	2.20	0.40
1:C:77:ASP:HA	1:C:153:SER:C	2.46	0.40
1:D:92:LYS:HB3	1:D:133:TRP:CE2	2.56	0.40
1:B:138:ILE:HA	1:B:139:PRO:HD2	1.70	0.40
1:D:90:ASP:C	1:D:91:ILE:HG22	2.47	0.40
1:A:66:SER:HB3	1:A:160:PHE:HB2	2.02	0.40
1:A:126:TYR:HE1	1:A:139:PRO:CG	2.34	0.40
1:B:92:LYS:HB2	1:B:133:TRP:CH2	2.57	0.40
1:D:27:MET:HE3	1:D:27:MET:N	2.37	0.40
1:D:77:ASP:OD2	1:D:77:ASP:C	2.65	0.40
1:D:111:ARG:HG2	1:D:113:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/205 (84%)	124 (72%)	36 (21%)	13 (8%)	1	9
1	B	172/205 (84%)	121 (70%)	34 (20%)	17 (10%)	0	6
1	C	171/205 (83%)	126 (74%)	35 (20%)	10 (6%)	1	13
1	D	171/205 (83%)	123 (72%)	31 (18%)	17 (10%)	0	6
All	All	687/820 (84%)	494 (72%)	136 (20%)	57 (8%)	0	7

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	A	82	VAL
1	A	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	141	ARG
1	A	147	ASN
1	A	165	ALA
1	B	83	GLU
1	B	84	ASN
1	B	141	ARG
1	B	147	ASN
1	C	79	SER
1	C	84	ASN
1	C	141	ARG
1	C	147	ASN
1	D	42	THR
1	D	79	SER
1	D	84	ASN
1	D	141	ARG
1	D	147	ASN
1	A	26	GLY
1	B	26	GLY
1	B	56	GLN
1	B	79	SER
1	B	82	VAL
1	B	134	GLN
1	B	140	LEU
1	B	144	MET
1	C	26	GLY
1	C	56	GLN
1	D	26	GLY
1	D	46	ASN
1	D	56	GLN
1	D	82	VAL
1	D	131	THR
1	D	134	GLN
1	A	16	ASP
1	A	89	PHE
1	A	131	THR
1	A	134	GLN
1	A	144	MET
1	B	27	MET
1	B	44	THR
1	C	134	GLN
1	C	144	MET
1	D	107	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	144	MET
1	B	61	SER
1	B	131	THR
1	D	16	ASP
1	A	7	LYS
1	B	42	THR
1	D	95	GLU
1	C	91	ILE
1	C	82	VAL
1	D	47	GLY
1	B	152	PRO
1	D	146	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	159/182 (87%)	111 (70%)	48 (30%)	0	2
1	B	158/182 (87%)	110 (70%)	48 (30%)	0	2
1	C	157/182 (86%)	100 (64%)	57 (36%)	0	1
1	D	157/182 (86%)	90 (57%)	67 (43%)	0	0
All	All	631/728 (87%)	411 (65%)	220 (35%)	0	2

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	LEU
1	A	11	VAL
1	A	14	PHE
1	A	19	VAL
1	A	32	THR
1	A	33	ILE
1	A	35	ASP
1	A	36	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	37	LEU
1	A	46	ASN
1	A	50	THR
1	A	51	LEU
1	A	55	VAL
1	A	57	THR
1	A	68	LEU
1	A	69	THR
1	A	71	ARG
1	A	75	THR
1	A	78	LEU
1	A	80	GLN
1	A	84	ASN
1	A	87	LEU
1	A	94	LYS
1	A	95	GLU
1	A	112	VAL
1	A	115	LEU
1	A	117	ILE
1	A	120	THR
1	A	121	THR
1	A	123	ILE
1	A	127	VAL
1	A	128	THR
1	A	129	VAL
1	A	132	ASP
1	A	136	VAL
1	A	140	LEU
1	A	142	ASP
1	A	146	ILE
1	A	157	CYS
1	A	158	LEU
1	A	161	SER
1	A	163	ARG
1	A	170	VAL
1	A	176	LYS
1	A	177	ILE
1	A	178	THR
1	A	180	GLU
1	B	8	LEU
1	B	11	VAL
1	B	13	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	14	PHE
1	B	19	VAL
1	B	20	VAL
1	B	23	SER
1	B	25	SER
1	B	29	GLU
1	B	39	VAL
1	B	41	THR
1	B	42	THR
1	B	46	ASN
1	B	48	LEU
1	B	53	LEU
1	B	55	VAL
1	B	57	THR
1	B	59	VAL
1	B	61	SER
1	B	65	ILE
1	B	67	LEU
1	B	68	LEU
1	B	74	ASN
1	B	75	THR
1	B	80	GLN
1	B	82	VAL
1	B	84	ASN
1	B	87	LEU
1	B	101	VAL
1	B	112	VAL
1	B	115	LEU
1	B	119	VAL
1	B	120	THR
1	B	121	THR
1	B	122	VAL
1	B	123	ILE
1	B	127	VAL
1	B	131	THR
1	B	143	LEU
1	B	148	ASN
1	B	155	VAL
1	B	158	LEU
1	B	162	LYS
1	B	170	VAL
1	B	176	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	177	ILE
1	B	178	THR
1	B	181	ASP
1	C	9	LEU
1	C	11	VAL
1	C	15	LYS
1	C	19	VAL
1	C	23	SER
1	C	25	SER
1	C	27	MET
1	C	32	THR
1	C	33	ILE
1	C	36	THR
1	C	37	LEU
1	C	41	THR
1	C	44	THR
1	C	50	THR
1	C	55	VAL
1	C	58	THR
1	C	60	GLN
1	C	65	ILE
1	C	67	LEU
1	C	71	ARG
1	C	75	THR
1	C	77	ASP
1	C	82	VAL
1	C	83	GLU
1	C	90	ASP
1	C	94	LYS
1	C	95	GLU
1	C	101	VAL
1	C	102	ILE
1	C	108	VAL
1	C	111	ARG
1	C	115	LEU
1	C	118	ASP
1	C	119	VAL
1	C	122	VAL
1	C	123	ILE
1	C	124	SER
1	C	126	TYR
1	C	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	128	THR
1	C	132	ASP
1	C	136	VAL
1	C	140	LEU
1	C	141	ARG
1	C	146	ILE
1	C	148	ASN
1	C	152	PRO
1	C	153	SER
1	C	155	VAL
1	C	156	THR
1	C	162	LYS
1	C	163	ARG
1	C	166	ASP
1	C	169	THR
1	C	175	ILE
1	C	176	LYS
1	C	180	GLU
1	D	9	LEU
1	D	11	VAL
1	D	19	VAL
1	D	20	VAL
1	D	27	MET
1	D	32	THR
1	D	33	ILE
1	D	35	ASP
1	D	36	THR
1	D	37	LEU
1	D	39	VAL
1	D	42	THR
1	D	43	VAL
1	D	50	THR
1	D	55	VAL
1	D	58	THR
1	D	59	VAL
1	D	60	GLN
1	D	61	SER
1	D	65	ILE
1	D	66	SER
1	D	71	ARG
1	D	74	ASN
1	D	77	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	79	SER
1	D	80	GLN
1	D	82	VAL
1	D	84	ASN
1	D	88	GLU
1	D	91	ILE
1	D	92	LYS
1	D	95	GLU
1	D	98	GLU
1	D	99	ASP
1	D	101	VAL
1	D	105	ARG
1	D	112	VAL
1	D	113	TYR
1	D	116	GLU
1	D	120	THR
1	D	121	THR
1	D	122	VAL
1	D	123	ILE
1	D	124	SER
1	D	127	VAL
1	D	128	THR
1	D	130	THR
1	D	132	ASP
1	D	136	VAL
1	D	137	LYS
1	D	138	ILE
1	D	140	LEU
1	D	141	ARG
1	D	142	ASP
1	D	144	MET
1	D	146	ILE
1	D	147	ASN
1	D	154	SER
1	D	158	LEU
1	D	161	SER
1	D	163	ARG
1	D	166	ASP
1	D	170	VAL
1	D	173	SER
1	D	175	ILE
1	D	176	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	178	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	54	ASN
1	A	60	GLN
1	A	80	GLN
1	A	84	ASN
1	A	125	ASN
1	A	147	ASN
1	B	54	ASN
1	B	74	ASN
1	B	80	GLN
1	B	84	ASN
1	B	125	ASN
1	C	54	ASN
1	C	80	GLN
1	C	125	ASN
1	C	134	GLN
1	C	135	HIS
1	C	148	ASN
1	D	12	GLN
1	D	54	ASN
1	D	56	GLN
1	D	135	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	175/205 (85%)	-0.53	0 100 100	9, 36, 52, 62	4 (2%)
1	B	174/205 (84%)	-0.60	1 (0%) 85 64	10, 36, 52, 58	4 (2%)
1	C	173/205 (84%)	-0.64	0 100 100	8, 36, 51, 57	4 (2%)
1	D	173/205 (84%)	-0.59	1 (0%) 85 64	10, 36, 51, 58	3 (1%)
All	All	695/820 (84%)	-0.59	2 (0%) 90 75	8, 36, 52, 62	15 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	GLY	2.3
1	B	61	SER	2.1

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 oligosaccharides 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.