



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 10:09 AM EDT

PDB ID : 4JAR
Title : Crystal structure of mycobacterium tuberculosis pks11 in complex with polyketide intermediates and evidence that it synthesizes ALKYL PYRONES
Authors : Gokulan, K.; Sacchettini, J.C.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on : 2013-02-19
Resolution : 1.98 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)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

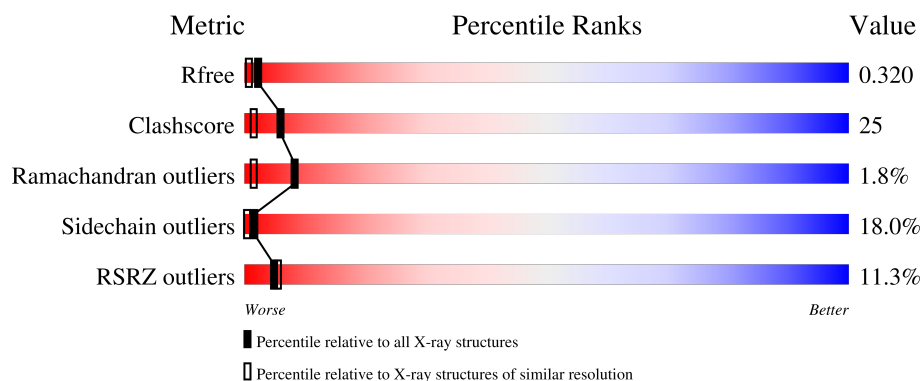
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	353	<div> <div>9%</div> <div>54%</div> <div>34%</div> <div>11%</div> <div>.</div> </div>
1	B	353	<div> <div>13%</div> <div>58%</div> <div>34%</div> <div>7%</div> <div>.</div> </div>
1	C	353	<div> <div>12%</div> <div>53%</div> <div>36%</div> <div>10%</div> </div>
1	D	353	<div> <div>11%</div> <div>56%</div> <div>35%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10576 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.

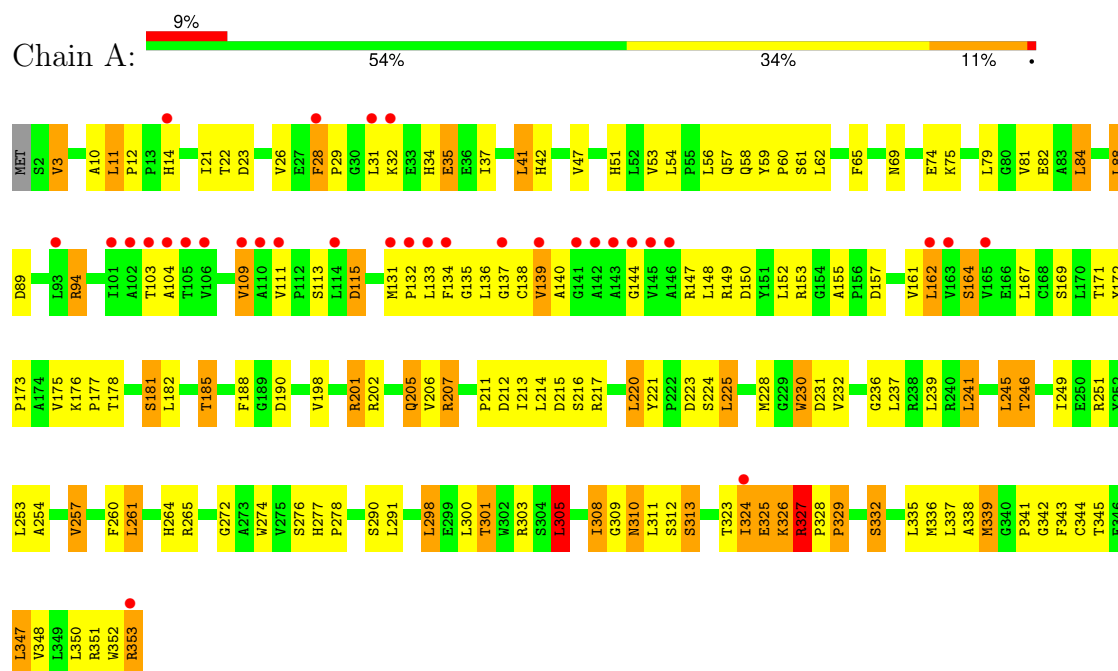
- Molecule 1 is a protein called Alpha-pyrone synthesis polyketide synthase-like Pks11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	C	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	B	353	Total	C	N	O	S	0	0	0
			2650	1676	470	495	9			
1	D	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			

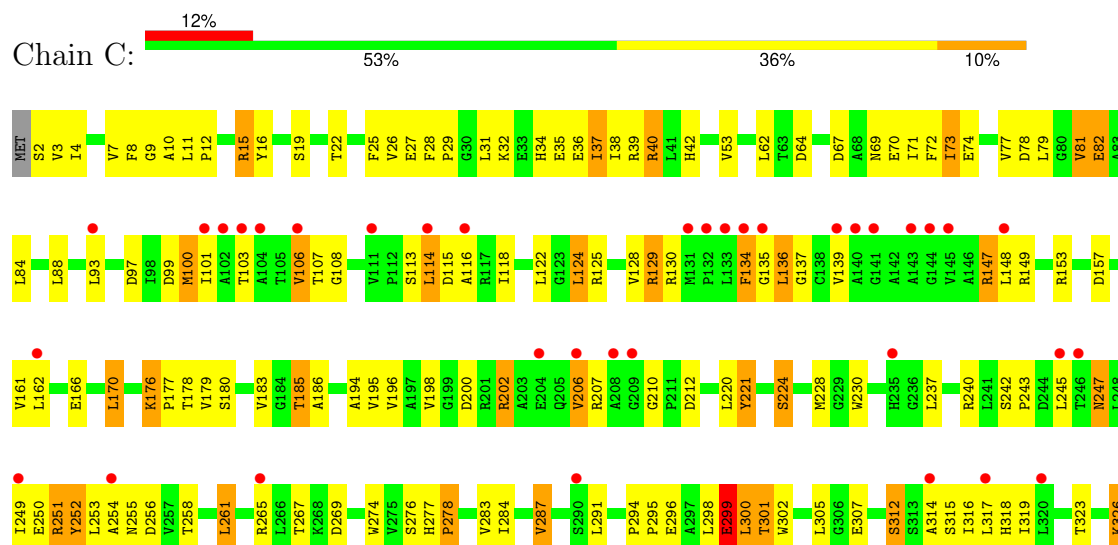
3 Residue-property plots

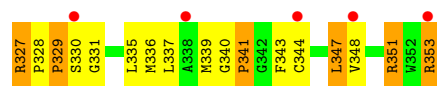
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-pyrone synthesis polyketide synthase-like Pks11

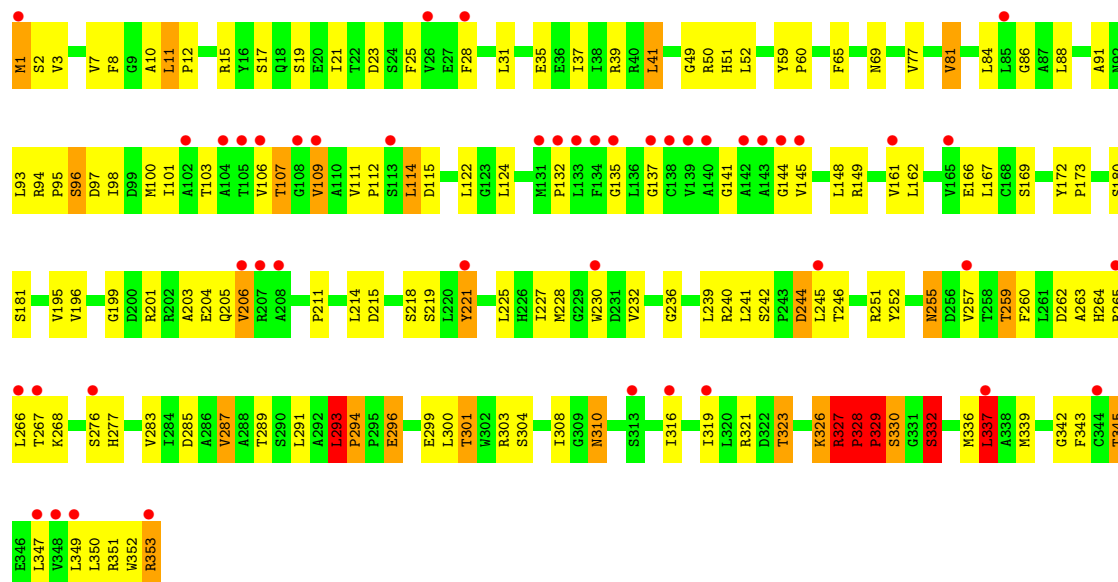


- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

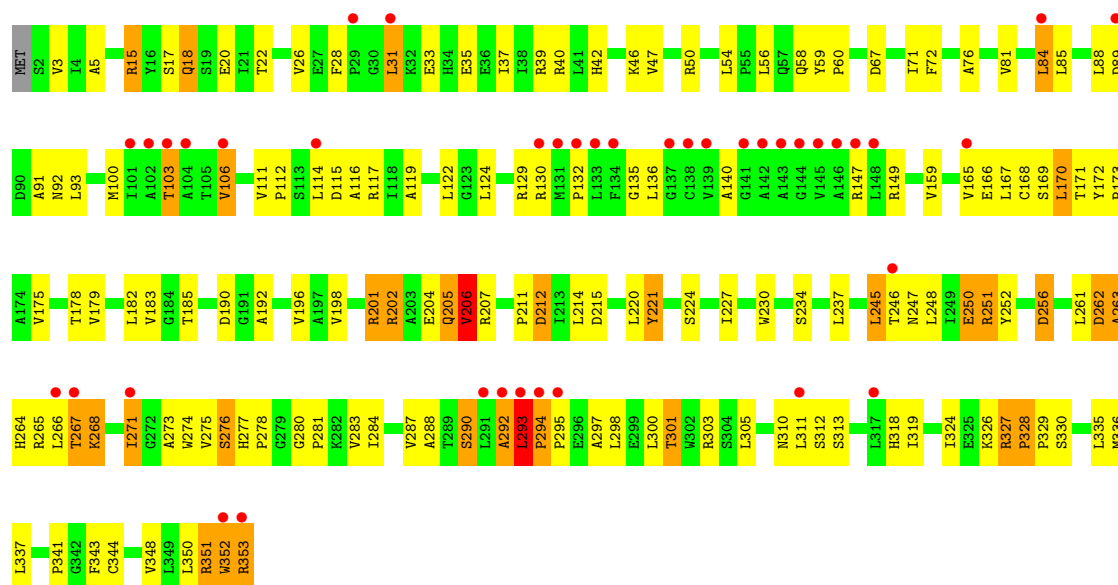




- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11



- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.60Å 48.52Å 195.23Å 90.00° 98.41° 90.00°	Depositor
Resolution (Å)	38.24 – 1.98 38.24 – 1.98	Depositor EDS
% Data completeness (in resolution range)	70.0 (38.24-1.98) 70.3 (38.24-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, R_{free}	0.268 , 0.314 0.306 , 0.320	Depositor DCC
R_{free} test set	3377 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10576	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.62	1/2695 (0.0%)	0.70	2/3671 (0.1%)
1	B	0.54	1/2703 (0.0%)	0.70	5/3681 (0.1%)
1	C	0.67	1/2695 (0.0%)	0.73	3/3671 (0.1%)
1	D	0.60	3/2695 (0.1%)	0.71	4/3671 (0.1%)
All	All	0.61	6/10788 (0.1%)	0.71	14/14694 (0.1%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	295	PRO	N-CD	5.52	1.55	1.47
1	D	328	PRO	N-CD	5.48	1.55	1.47
1	D	294	PRO	N-CD	5.41	1.55	1.47
1	A	29	PRO	N-CD	5.34	1.55	1.47
1	B	328	PRO	N-CD	5.19	1.55	1.47
1	C	329	PRO	N-CD	5.06	1.54	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	PRO	C-N-CD	6.54	142.13	128.40
1	C	294	PRO	C-N-CD	6.04	141.08	128.40
1	C	328	PRO	C-N-CD	5.82	140.61	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	328	PRO	C-N-CD	5.78	140.53	128.40
1	D	327	ARG	C-N-CD	5.73	140.43	128.40
1	C	327	ARG	C-N-CD	5.72	140.42	128.40
1	B	327	ARG	C-N-CD	5.69	140.35	128.40
1	B	337	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	293	LEU	C-N-CD	5.54	140.04	128.40
1	B	329	PRO	CA-N-CD	-5.52	103.78	111.50
1	A	28	PHE	C-N-CD	5.50	139.96	128.40
1	D	293	LEU	C-N-CD	5.45	139.85	128.40
1	D	294	PRO	C-N-CD	5.18	139.29	128.40
1	A	305	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	GLY	Peptide
1	B	2	SER	Peptide
1	C	344	CYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2642	0	2675	146	0
1	B	2650	0	2687	124	0
1	C	2642	0	2675	121	1
1	D	2642	0	2675	157	1
All	All	10576	0	10712	531	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 25.

All (531) 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:28:PHE:HB2	1:B:31:LEU:CD1	1.46	1.44
1:C:251:ARG:HG2	1:C:252:TYR:CE1	1.59	1.38
1:A:300:LEU:CD1	1:A:323:THR:HG22	1.58	1.34
1:B:28:PHE:CB	1:B:31:LEU:HD12	1.70	1.22
1:B:84:LEU:HD23	1:B:122:LEU:CD1	1.70	1.21
1:D:26:VAL:HG11	1:D:35:GLU:HG3	1.21	1.20
1:C:37:ILE:HD12	1:C:40:ARG:HH21	1.00	1.14
1:B:28:PHE:CB	1:B:31:LEU:CD1	2.26	1.13
1:B:84:LEU:HD23	1:B:122:LEU:HD13	1.14	1.12
1:C:296:GLU:HB2	1:C:299:GLU:OE2	1.49	1.12
1:D:353:ARG:HG2	1:D:353:ARG:HH21	1.16	1.09
1:B:329:PRO:HD2	1:B:332:SER:OG	1.51	1.09
1:A:94:ARG:HH21	1:A:94:ARG:HG3	1.17	1.09
1:C:84:LEU:HD23	1:C:122:LEU:CD1	1.82	1.08
1:D:353:ARG:HH21	1:D:353:ARG:CG	1.65	1.07
1:C:84:LEU:HD23	1:C:122:LEU:HD12	1.08	1.06
1:C:37:ILE:HD12	1:C:40:ARG:NH2	1.69	1.06
1:A:300:LEU:HD13	1:A:323:THR:HG22	1.35	1.05
1:A:300:LEU:HD13	1:A:323:THR:CG2	1.89	1.03
1:A:353:ARG:OXT	1:A:353:ARG:HG2	1.52	1.02
1:B:28:PHE:HB2	1:B:31:LEU:HD12	1.12	1.02
1:D:26:VAL:CG1	1:D:35:GLU:HG3	1.89	1.02
1:A:300:LEU:HD12	1:A:323:THR:HG22	1.40	1.02
1:D:352:TRP:O	1:D:353:ARG:HB2	1.56	1.01
1:A:353:ARG:HH11	1:A:353:ARG:HB2	1.25	1.01
1:D:252:TYR:O	1:D:256:ASP:OD1	1.82	0.98
1:D:26:VAL:HG11	1:D:35:GLU:CG	1.93	0.97
1:D:42:HIS:NE2	1:D:185:THR:HG23	1.80	0.96
1:A:300:LEU:CD1	1:A:323:THR:CG2	2.43	0.96
1:C:251:ARG:CG	1:C:252:TYR:CE1	2.48	0.96
1:D:275:VAL:HG12	1:D:275:VAL:O	1.66	0.95
1:C:84:LEU:CD2	1:C:122:LEU:HD12	1.99	0.92
1:A:336:MET:HB2	1:A:348:VAL:HB	1.49	0.92
1:D:182:LEU:O	1:D:185:THR:HG22	1.71	0.91
1:C:125:ARG:O	1:C:128:VAL:HG12	1.69	0.91
1:B:28:PHE:HB2	1:B:31:LEU:HD13	1.49	0.91
1:D:274:TRP:CH2	1:D:335:LEU:HD23	2.06	0.91
1:D:204:GLU:O	1:D:205:GLN:HB2	1.71	0.90
1:B:245:LEU:HD11	1:B:343:PHE:CE1	2.06	0.90
1:D:274:TRP:CZ3	1:D:335:LEU:HD23	2.07	0.89
1:D:273:ALA:HB2	1:D:352:TRP:HE1	1.38	0.87
1:B:107:THR:HG21	1:B:167:LEU:H	1.38	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:VAL:HG12	1:D:336:MET:HA	1.55	0.87
1:A:34:HIS:CD2	1:A:177:PRO:HB3	2.09	0.87
1:D:353:ARG:HH21	1:D:353:ARG:CB	1.88	0.86
1:D:273:ALA:CB	1:D:352:TRP:HE1	1.88	0.86
1:A:353:ARG:HH11	1:A:353:ARG:CB	1.89	0.86
1:A:42:HIS:NE2	1:A:185:THR:HG22	1.92	0.84
1:C:206:VAL:HG13	1:C:206:VAL:O	1.77	0.84
1:C:166:GLU:HG3	1:C:312:SER:HB3	1.59	0.83
1:D:265:ARG:O	1:D:266:LEU:HG	1.78	0.83
1:B:327:ARG:HH21	1:B:327:ARG:HG3	1.44	0.83
1:D:192:ALA:O	1:D:318:HIS:HE1	1.60	0.82
1:C:251:ARG:HG2	1:C:252:TYR:CZ	2.14	0.82
1:A:232:VAL:HG21	1:B:109:VAL:HG22	1.62	0.82
1:A:311:LEU:HD12	1:A:311:LEU:N	1.93	0.82
1:B:201:ARG:HD2	1:D:353:ARG:HG2	1.60	0.81
1:D:353:ARG:HG2	1:D:353:ARG:NH2	1.87	0.81
1:B:84:LEU:CD2	1:B:122:LEU:HD13	2.05	0.81
1:C:73:ILE:HD12	1:C:73:ILE:O	1.79	0.80
1:C:28:PHE:O	1:C:31:LEU:HB2	1.81	0.80
1:D:275:VAL:O	1:D:275:VAL:CG1	2.30	0.80
1:A:69:ASN:HD21	1:A:109:VAL:H	1.28	0.79
1:C:206:VAL:O	1:C:206:VAL:CG1	2.30	0.79
1:A:337:LEU:HD23	1:A:338:ALA:N	1.97	0.79
1:B:59:TYR:CE2	1:B:169:SER:HB3	2.18	0.79
1:D:59:TYR:CE2	1:D:169:SER:HB2	2.17	0.78
1:A:326:LYS:C	1:A:327:ARG:HG3	2.02	0.78
1:C:113:SER:HB3	1:D:135:GLY:HA3	1.66	0.78
1:D:81:VAL:HG12	1:D:85:LEU:HD12	1.65	0.78
1:B:285:ASP:O	1:B:289:THR:OG1	2.00	0.78
1:D:353:ARG:CG	1:D:353:ARG:NH2	2.37	0.78
1:C:42:HIS:NE2	1:C:185:THR:HG22	1.98	0.77
1:A:178:THR:CG2	1:A:181:SER:HB2	2.15	0.77
1:A:220:LEU:HD23	1:A:344:CYS:HB3	1.67	0.77
1:A:94:ARG:HG3	1:A:94:ARG:NH2	1.98	0.77
1:D:251:ARG:HB3	1:D:252:TYR:CD1	2.20	0.76
1:A:94:ARG:HH21	1:A:94:ARG:CG	1.97	0.76
1:B:93:LEU:HD21	1:B:206:VAL:HG11	1.68	0.76
1:D:352:TRP:O	1:D:353:ARG:CB	2.32	0.75
1:A:111:VAL:HG22	1:B:135:GLY:HA2	1.68	0.75
1:D:277:HIS:ND1	1:D:278:PRO:HD2	2.02	0.75
1:C:135:GLY:HA2	1:D:111:VAL:HG22	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ARG:C	1:D:266:LEU:HG	2.08	0.75
1:D:202:ARG:C	1:D:204:GLU:H	1.89	0.74
1:A:276:SER:HB3	1:A:301:THR:HG21	1.70	0.74
1:C:116:ALA:HB2	1:C:130:ARG:NH1	2.01	0.74
1:C:298:LEU:O	1:C:299:GLU:C	2.24	0.74
1:A:178:THR:HG23	1:A:181:SER:H	1.53	0.74
1:A:337:LEU:HD23	1:A:337:LEU:C	2.08	0.73
1:A:35:GLU:O	1:A:35:GLU:HG3	1.89	0.73
1:B:214:LEU:HD11	1:B:351:ARG:HB2	1.71	0.72
1:C:73:ILE:HD12	1:C:73:ILE:C	2.09	0.72
1:A:310:ASN:C	1:A:311:LEU:HD12	2.09	0.72
1:A:257:VAL:HG23	1:A:261:LEU:HD22	1.72	0.72
1:B:201:ARG:CD	1:D:353:ARG:HG2	2.20	0.71
1:A:214:LEU:O	1:A:215:ASP:HB2	1.89	0.71
1:C:253:LEU:HD23	1:C:291:LEU:HD21	1.72	0.71
1:A:311:LEU:N	1:A:311:LEU:CD1	2.55	0.70
1:C:42:HIS:NE2	1:C:185:THR:CG2	2.54	0.70
1:B:107:THR:HG21	1:B:167:LEU:N	2.05	0.70
1:D:353:ARG:CB	1:D:353:ARG:NH2	2.53	0.70
1:A:310:ASN:C	1:A:310:ASN:HD22	1.94	0.70
1:B:227:ILE:HG21	1:B:245:LEU:HD13	1.73	0.70
1:C:299:GLU:O	1:C:301:THR:N	2.25	0.70
1:B:227:ILE:CG2	1:B:245:LEU:HD13	2.23	0.69
1:B:1:MET:H1	1:B:149:ARG:HE	1.39	0.69
1:D:202:ARG:C	1:D:204:GLU:N	2.44	0.69
1:D:268:LYS:O	1:D:268:LYS:CG	2.40	0.69
1:A:34:HIS:NE2	1:A:177:PRO:HB3	2.07	0.69
1:D:268:LYS:O	1:D:268:LYS:HG3	1.91	0.69
1:C:22:THR:O	1:C:26:VAL:HG13	1.94	0.68
1:C:67:ASP:O	1:C:71:ILE:HG13	1.93	0.68
1:B:327:ARG:HG3	1:B:327:ARG:NH2	2.07	0.68
1:D:261:LEU:O	1:D:266:LEU:O	2.10	0.68
1:D:330:SER:OG	1:D:353:ARG:HD3	1.92	0.68
1:C:136:LEU:HD12	1:D:130:ARG:NH2	2.09	0.68
1:B:94:ARG:HG2	1:B:97:ASP:OD2	1.93	0.68
1:A:32:LYS:O	1:A:32:LYS:HG3	1.93	0.68
1:D:250:GLU:HA	1:D:290:SER:OG	1.94	0.68
1:B:69:ASN:HD21	1:B:109:VAL:H	1.40	0.68
1:D:335:LEU:HD12	1:D:348:VAL:O	1.94	0.67
1:A:149:ARG:HD2	1:A:213:ILE:HG22	1.75	0.67
1:A:178:THR:O	1:A:182:LEU:HG	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:HIS:ND1	1:A:278:PRO:HD2	2.09	0.67
1:B:106:VAL:HG22	1:B:230:TRP:HE1	1.58	0.67
1:A:274:TRP:CZ3	1:A:335:LEU:HD23	2.28	0.67
1:C:116:ALA:HB2	1:C:130:ARG:HH11	1.59	0.67
1:A:353:ARG:HH11	1:A:353:ARG:CG	2.06	0.67
1:D:330:SER:OG	1:D:353:ARG:CD	2.43	0.67
1:B:329:PRO:HD2	1:B:332:SER:HG	1.59	0.67
1:D:93:LEU:HD21	1:D:206:VAL:HG21	1.77	0.66
1:C:267:THR:HG23	1:C:269:ASP:H	1.60	0.66
1:A:169:SER:OG	1:A:190:ASP:OD2	2.13	0.66
1:D:353:ARG:HH21	1:D:353:ARG:HB3	1.61	0.66
1:A:205:GLN:O	1:A:205:GLN:HG2	1.95	0.66
1:C:296:GLU:N	1:C:296:GLU:OE1	2.26	0.66
1:D:81:VAL:HG13	1:D:122:LEU:HD21	1.78	0.66
1:D:352:TRP:HA	1:D:352:TRP:CE3	2.30	0.65
1:C:32:LYS:NZ	1:C:35:GLU:OE1	2.20	0.65
1:A:59:TYR:N	1:A:60:PRO:HD2	2.12	0.64
1:D:179:VAL:O	1:D:183:VAL:HG23	1.97	0.64
1:A:53:VAL:HG13	1:A:54:LEU:HD13	1.79	0.64
1:C:296:GLU:CB	1:C:299:GLU:OE2	2.38	0.64
1:C:299:GLU:O	1:C:302:TRP:N	2.30	0.64
1:A:167:LEU:HD23	1:A:190:ASP:HB3	1.80	0.64
1:A:353:ARG:OXT	1:A:353:ARG:CG	2.30	0.64
1:D:72:PHE:HA	1:D:170:LEU:HD23	1.78	0.64
1:A:217:ARG:HB2	1:A:260:PHE:CD1	2.32	0.64
1:A:264:HIS:CE1	1:D:201:ARG:HG3	2.33	0.63
1:C:26:VAL:HG23	1:C:27:GLU:OE1	1.98	0.63
1:A:353:ARG:HB2	1:A:353:ARG:NH1	2.06	0.63
1:C:2:SER:OG	1:C:149:ARG:HA	1.99	0.63
1:D:192:ALA:O	1:D:318:HIS:CE1	2.48	0.63
1:D:265:ARG:O	1:D:266:LEU:CG	2.46	0.62
1:D:103:THR:HB	1:D:115:ASP:HB3	1.82	0.62
1:A:300:LEU:HD13	1:A:323:THR:HG23	1.76	0.62
1:A:206:VAL:C	1:A:207:ARG:HG2	2.18	0.62
1:C:179:VAL:O	1:C:183:VAL:HG23	1.99	0.62
1:A:11:LEU:HD23	1:A:51:HIS:NE2	2.14	0.62
1:D:26:VAL:HG11	1:D:35:GLU:CD	2.20	0.62
1:B:283:VAL:O	1:B:287:VAL:CG1	2.48	0.62
1:D:22:THR:O	1:D:26:VAL:HG23	2.00	0.62
1:D:288:ALA:O	1:D:292:ALA:HA	1.99	0.62
1:D:301:THR:HB	1:D:319:ILE:HD13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:VAL:HG11	1:D:336:MET:HG2	1.82	0.61
1:D:59:TYR:HE2	1:D:169:SER:HB2	1.66	0.61
1:A:225:LEU:HD13	1:A:225:LEU:N	2.15	0.61
1:A:310:ASN:ND2	1:A:312:SER:H	1.98	0.61
1:B:296:GLU:OE2	1:B:296:GLU:N	2.32	0.61
1:C:283:VAL:O	1:C:287:VAL:HG12	2.00	0.61
1:B:91:ALA:O	1:B:93:LEU:HG	2.01	0.61
1:C:252:TYR:N	1:C:252:TYR:CD1	2.69	0.61
1:B:28:PHE:HB3	1:B:31:LEU:HD12	1.77	0.60
1:D:211:PRO:HG3	1:D:352:TRP:CZ3	2.36	0.60
1:C:224:SER:HB3	1:C:343:PHE:H	1.65	0.60
1:D:262:ASP:C	1:D:264:HIS:N	2.52	0.60
1:B:328:PRO:HB3	1:B:329:PRO:HD3	1.83	0.60
1:B:245:LEU:CD1	1:B:343:PHE:CE1	2.84	0.60
1:A:254:ALA:HA	1:A:291:LEU:HD21	1.82	0.60
1:D:76:ALA:HB1	1:D:165:VAL:HG11	1.83	0.60
1:B:25:PHE:O	1:B:31:LEU:HD13	2.02	0.60
1:A:225:LEU:HD13	1:A:225:LEU:H	1.66	0.59
1:C:25:PHE:CE2	1:C:185:THR:HG21	2.37	0.59
1:A:178:THR:HG22	1:A:181:SER:HB2	1.83	0.59
1:B:225:LEU:HD23	1:B:342:GLY:O	2.03	0.59
1:D:262:ASP:C	1:D:264:HIS:H	2.05	0.59
1:B:326:LYS:O	1:B:326:LYS:HG3	2.03	0.59
1:A:225:LEU:N	1:A:225:LEU:CD1	2.66	0.59
1:B:59:TYR:HE2	1:B:169:SER:HB3	1.66	0.58
1:B:103:THR:HG21	1:B:114:LEU:HB2	1.83	0.58
1:A:10:ALA:O	1:A:11:LEU:HD12	2.03	0.58
1:D:328:PRO:HG2	1:D:352:TRP:CG	2.38	0.58
1:B:49:GLY:O	1:B:50:ARG:HG3	2.03	0.58
1:B:94:ARG:O	1:B:97:ASP:HB2	2.02	0.58
1:B:260:PHE:CE2	1:B:349:LEU:HB2	2.38	0.58
1:A:136:LEU:HB2	1:A:140:ALA:HB2	1.86	0.58
1:C:93:LEU:HB3	1:C:97:ASP:OD2	2.02	0.58
1:C:330:SER:HB3	1:C:353:ARG:HG3	1.86	0.58
1:C:147:ARG:HH12	1:D:129:ARG:HH21	1.51	0.58
1:B:283:VAL:O	1:B:287:VAL:HG13	2.04	0.57
1:D:262:ASP:O	1:D:264:HIS:N	2.38	0.57
1:B:319:ILE:O	1:B:323:THR:HG22	2.04	0.57
1:D:251:ARG:HB3	1:D:252:TYR:CE1	2.38	0.57
1:D:15:ARG:HH21	1:D:15:ARG:HG3	1.69	0.57
1:D:294:PRO:HD2	1:D:297:ALA:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PHE:CG	1:B:236:GLY:HA2	2.40	0.57
1:A:150:ASP:OD1	1:A:153:ARG:NH1	2.37	0.57
1:A:56:LEU:HD12	1:A:56:LEU:O	2.05	0.56
1:D:26:VAL:CG1	1:D:35:GLU:CG	2.69	0.56
1:D:26:VAL:HG11	1:D:35:GLU:OE2	2.06	0.56
1:D:47:VAL:HG22	1:D:305:LEU:O	2.05	0.56
1:C:62:LEU:HD11	1:C:170:LEU:HD12	1.87	0.56
1:B:149:ARG:NH2	1:B:215:ASP:HA	2.20	0.56
1:A:11:LEU:HD21	1:A:308:ILE:HD11	1.88	0.56
1:A:84:LEU:O	1:A:88:LEU:HB2	2.05	0.56
1:C:274:TRP:CZ3	1:C:335:LEU:HD23	2.41	0.56
1:D:116:ALA:HB2	1:D:130:ARG:NH1	2.20	0.56
1:D:167:LEU:HB3	1:D:170:LEU:HD22	1.88	0.56
1:A:328:PRO:O	1:A:329:PRO:C	2.42	0.56
1:C:277:HIS:ND1	1:C:278:PRO:HD2	2.21	0.56
1:C:251:ARG:HG2	1:C:252:TYR:HE1	1.56	0.56
1:B:8:PHE:CD2	1:B:86:GLY:HA3	2.41	0.56
1:D:353:ARG:NH2	1:D:353:ARG:HB3	2.20	0.56
1:B:28:PHE:HB3	1:B:31:LEU:CD1	2.31	0.55
1:D:256:ASP:OD1	1:D:256:ASP:N	2.38	0.55
1:D:328:PRO:CG	1:D:352:TRP:CG	2.89	0.55
1:A:94:ARG:NH2	1:A:94:ARG:CG	2.62	0.55
1:D:15:ARG:HH21	1:D:15:ARG:CG	2.18	0.55
1:D:28:PHE:CZ	1:D:60:PRO:HD3	2.41	0.55
1:B:35:GLU:OE1	1:B:39:ARG:NH1	2.40	0.55
1:B:141:GLY:O	1:B:145:VAL:HG23	2.07	0.55
1:D:93:LEU:CD2	1:D:206:VAL:HG21	2.36	0.55
1:C:161:VAL:HG12	1:C:196:VAL:HG22	1.88	0.55
1:D:271:ILE:HD12	1:D:271:ILE:C	2.27	0.55
1:C:137:GLY:O	1:C:139:VAL:N	2.40	0.55
1:B:28:PHE:CB	1:B:31:LEU:HD11	2.32	0.54
1:D:324:ILE:HG12	1:D:352:TRP:CZ3	2.41	0.54
1:B:1:MET:N	1:B:149:ARG:HE	2.05	0.54
1:D:81:VAL:HG12	1:D:85:LEU:CD1	2.34	0.54
1:D:328:PRO:HG3	1:D:352:TRP:CD2	2.42	0.54
1:B:7:VAL:CG1	1:B:321:ARG:HB2	2.37	0.54
1:A:337:LEU:C	1:A:337:LEU:CD2	2.75	0.54
1:D:3:VAL:HA	1:D:212:ASP:HA	1.89	0.54
1:D:18:GLN:HE21	1:D:18:GLN:HA	1.71	0.54
1:A:22:THR:O	1:A:26:VAL:HG13	2.08	0.54
1:C:134:PHE:CD1	1:C:134:PHE:C	2.81	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:PHE:CZ	1:B:349:LEU:HB2	2.43	0.54
1:A:253:LEU:HD11	1:A:337:LEU:HD11	1.89	0.54
1:B:337:LEU:HB2	1:B:347:LEU:HD23	1.90	0.54
1:D:28:PHE:HB2	1:D:31:LEU:HD11	1.89	0.53
1:D:271:ILE:HD11	1:D:274:TRP:CD1	2.43	0.53
1:B:255:ASN:O	1:B:259:THR:HG23	2.08	0.53
1:A:239:LEU:HD21	1:A:241:LEU:HD12	1.89	0.53
1:A:109:VAL:HG22	1:B:232:VAL:HG21	1.91	0.53
1:A:21:ILE:HA	1:A:56:LEU:HD21	1.91	0.53
1:A:308:ILE:HG23	1:A:311:LEU:HD21	1.91	0.53
1:A:157:ASP:CG	1:A:201:ARG:HE	2.12	0.53
1:A:221:TYR:O	1:A:224:SER:OG	2.26	0.53
1:C:337:LEU:HD13	1:C:347:LEU:CD1	2.39	0.53
1:A:337:LEU:HG	1:A:347:LEU:HD11	1.90	0.52
1:A:69:ASN:HD21	1:A:109:VAL:N	2.01	0.52
1:C:38:ILE:O	1:C:39:ARG:C	2.46	0.52
1:B:59:TYR:N	1:B:60:PRO:CD	2.73	0.52
1:D:220:LEU:HD12	1:D:343:PHE:O	2.09	0.52
1:A:230:TRP:HA	1:A:230:TRP:CE3	2.45	0.52
1:C:106:VAL:HG22	1:C:230:TRP:HE1	1.74	0.52
1:C:176:LYS:HB2	1:C:177:PRO:HD2	1.92	0.52
1:B:337:LEU:O	1:B:337:LEU:HD12	2.10	0.52
1:D:245:LEU:HD12	1:D:343:PHE:CE1	2.45	0.52
1:B:106:VAL:HG22	1:B:106:VAL:O	2.10	0.52
1:A:42:HIS:NE2	1:A:185:THR:CG2	2.70	0.52
1:C:4:ILE:O	1:C:210:GLY:HA3	2.10	0.51
1:C:42:HIS:CD2	1:C:186:ALA:HB2	2.45	0.51
1:B:37:ILE:HG12	1:B:41:LEU:HD22	1.93	0.51
1:D:267:THR:OG1	1:D:268:LYS:N	2.44	0.51
1:D:93:LEU:HD12	1:D:196:VAL:HG11	1.93	0.51
1:C:12:PRO:HD3	1:C:79:LEU:HD21	1.92	0.51
1:C:298:LEU:O	1:C:299:GLU:O	2.29	0.51
1:D:214:LEU:HD11	1:D:351:ARG:HB2	1.93	0.51
1:C:72:PHE:CD2	1:C:108:GLY:HA3	2.45	0.51
1:B:251:ARG:NH2	1:B:252:TYR:HE2	2.08	0.51
1:A:34:HIS:NE2	1:A:177:PRO:CB	2.74	0.50
1:C:124:LEU:HD23	1:C:124:LEU:N	2.27	0.50
1:A:152:LEU:O	1:A:155:ALA:O	2.29	0.50
1:D:172:TYR:N	1:D:173:PRO:HD2	2.27	0.50
1:B:337:LEU:HB2	1:B:347:LEU:CD2	2.41	0.50
1:D:140:ALA:HB3	1:D:313:SER:CB	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:TYR:HA	1:D:175:VAL:HG23	1.94	0.50
1:A:214:LEU:HD11	1:A:351:ARG:HB2	1.93	0.50
1:A:310:ASN:C	1:A:310:ASN:ND2	2.65	0.50
1:C:277:HIS:HB2	1:C:316:ILE:HD12	1.92	0.50
1:C:330:SER:CB	1:C:353:ARG:HG3	2.41	0.50
1:A:211:PRO:HD3	1:A:324:ILE:HD11	1.94	0.50
1:C:253:LEU:O	1:C:256:ASP:N	2.44	0.50
1:C:249:ILE:C	1:C:251:ARG:H	2.15	0.50
1:A:221:TYR:N	1:A:221:TYR:CD1	2.80	0.50
1:A:300:LEU:HD12	1:A:323:THR:CG2	2.28	0.49
1:D:76:ALA:CB	1:D:165:VAL:HG11	2.42	0.49
1:B:65:PHE:CD1	1:B:236:GLY:HA2	2.47	0.49
1:A:28:PHE:O	1:A:31:LEU:HB2	2.12	0.49
1:A:140:ALA:HB3	1:A:313:SER:HB2	1.95	0.49
1:B:52:LEU:HD22	1:B:169:SER:OG	2.12	0.49
1:D:212:ASP:OD1	1:D:212:ASP:N	2.45	0.49
1:A:198:VAL:HG13	1:A:202:ARG:HG2	1.93	0.49
1:C:251:ARG:CG	1:C:252:TYR:CD1	2.95	0.49
1:B:10:ALA:C	1:B:11:LEU:HG	2.33	0.49
1:A:172:TYR:HA	1:A:175:VAL:HG13	1.94	0.49
1:A:337:LEU:HG	1:A:347:LEU:CD1	2.42	0.49
1:C:267:THR:HG23	1:C:269:ASP:N	2.26	0.49
1:C:330:SER:CB	1:C:353:ARG:HB2	2.42	0.49
1:D:278:PRO:HA	1:D:284:ILE:HD11	1.93	0.49
1:D:337:LEU:HD23	1:D:337:LEU:C	2.33	0.49
1:A:169:SER:O	1:A:172:TYR:HB2	2.13	0.49
1:A:277:HIS:CE1	1:A:278:PRO:HD2	2.47	0.49
1:A:11:LEU:HD23	1:A:51:HIS:CD2	2.48	0.49
1:A:58:GLN:C	1:A:60:PRO:HD2	2.33	0.49
1:C:77:VAL:O	1:C:78:ASP:C	2.51	0.49
1:B:337:LEU:CB	1:B:347:LEU:HD23	2.42	0.49
1:A:308:ILE:O	1:A:311:LEU:HD11	2.13	0.49
1:D:59:TYR:N	1:D:60:PRO:HD2	2.28	0.49
1:A:221:TYR:N	1:A:221:TYR:HD1	2.11	0.48
1:A:310:ASN:HD22	1:A:312:SER:H	1.59	0.48
1:A:342:GLY:N	1:A:343:PHE:HA	2.28	0.48
1:D:136:LEU:O	1:D:341:PRO:HD2	2.13	0.48
1:C:298:LEU:O	1:C:301:THR:N	2.36	0.48
1:A:14:HIS:H	1:A:14:HIS:CD2	2.30	0.48
1:C:100:MET:CB	1:C:129:ARG:HB2	2.44	0.48
1:D:5:ALA:HB1	1:D:91:ALA:HB1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HB3	1:A:164:SER:HB2	1.95	0.48
1:C:3:VAL:HG22	1:C:212:ASP:OD1	2.13	0.48
1:B:227:ILE:HG21	1:B:245:LEU:CD1	2.42	0.48
1:D:28:PHE:CE1	1:D:60:PRO:HD3	2.49	0.48
1:B:94:ARG:HG3	1:B:96:SER:OG	2.14	0.48
1:A:329:PRO:HB2	1:A:332:SER:HB3	1.95	0.48
1:A:353:ARG:CG	1:A:353:ARG:NH1	2.72	0.48
1:C:3:VAL:O	1:C:198:VAL:HG12	2.13	0.48
1:B:28:PHE:CA	1:B:31:LEU:HD12	2.40	0.48
1:C:331:GLY:O	1:C:351:ARG:HD3	2.14	0.48
1:B:304:SER:O	1:B:308:ILE:HG12	2.14	0.48
1:D:276:SER:OG	1:D:277:HIS:N	2.47	0.48
1:A:59:TYR:CE2	1:A:169:SER:HB2	2.49	0.48
1:A:81:VAL:HG12	1:A:82:GLU:N	2.29	0.48
1:A:328:PRO:O	1:A:329:PRO:O	2.32	0.48
1:B:291:LEU:HB2	1:B:293:LEU:HD22	1.95	0.48
1:D:273:ALA:HB2	1:D:352:TRP:NE1	2.17	0.48
1:A:310:ASN:HD22	1:A:311:LEU:N	2.12	0.47
1:B:23:ASP:OD1	1:B:39:ARG:NH2	2.47	0.47
1:B:299:GLU:O	1:B:303:ARG:HG3	2.14	0.47
1:A:171:THR:C	1:A:173:PRO:HD2	2.34	0.47
1:C:34:HIS:O	1:C:35:GLU:C	2.53	0.47
1:C:147:ARG:HD3	1:C:147:ARG:HA	1.61	0.47
1:B:283:VAL:O	1:B:287:VAL:HG12	2.14	0.47
1:A:336:MET:CB	1:A:348:VAL:HB	2.34	0.47
1:D:26:VAL:HG13	1:D:35:GLU:HG3	1.90	0.47
1:D:149:ARG:NH1	1:D:215:ASP:OD1	2.47	0.47
1:C:198:VAL:HG22	1:C:202:ARG:HB3	1.95	0.47
1:B:115:ASP:OD2	1:B:132:PRO:HB3	2.15	0.47
1:D:328:PRO:HG3	1:D:352:TRP:CG	2.49	0.47
1:C:70:GLU:O	1:C:74:GLU:HG3	2.14	0.47
1:C:340:GLY:O	1:C:341:PRO:C	2.53	0.47
1:B:7:VAL:HG12	1:B:321:ARG:HB2	1.97	0.47
1:B:219:SER:HB3	1:B:345:THR:HG22	1.96	0.47
1:B:262:ASP:C	1:B:264:HIS:H	2.18	0.47
1:D:106:VAL:HG22	1:D:230:TRP:HE1	1.79	0.47
1:D:204:GLU:O	1:D:205:GLN:CB	2.54	0.47
1:A:144:GLY:HA3	1:A:162:LEU:HD13	1.97	0.47
1:B:201:ARG:CD	1:D:353:ARG:CG	2.92	0.47
1:D:84:LEU:HD13	1:D:122:LEU:HD12	1.97	0.47
1:A:74:GLU:HG2	1:A:75:LYS:N	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:CD2	1:C:122:LEU:CD1	2.73	0.46
1:C:319:ILE:HG22	1:C:319:ILE:O	2.14	0.46
1:D:328:PRO:HG3	1:D:352:TRP:CE2	2.50	0.46
1:B:3:VAL:HG11	1:B:203:ALA:CB	2.45	0.46
1:D:202:ARG:O	1:D:204:GLU:N	2.48	0.46
1:D:246:THR:O	1:D:250:GLU:HG2	2.16	0.46
1:A:230:TRP:HA	1:A:230:TRP:HE3	1.80	0.46
1:B:59:TYR:CZ	1:B:169:SER:HB3	2.48	0.46
1:B:336:MET:HG3	1:B:350:LEU:HD11	1.97	0.46
1:D:119:ALA:HA	1:D:124:LEU:HG	1.97	0.46
1:A:254:ALA:HA	1:A:291:LEU:CD2	2.45	0.46
1:C:53:VAL:HG11	1:C:170:LEU:HD22	1.96	0.46
1:D:17:SER:OG	1:D:20:GLU:HG3	2.16	0.46
1:D:265:ARG:O	1:D:266:LEU:CD2	2.64	0.46
1:A:324:ILE:O	1:A:327:ARG:N	2.48	0.46
1:D:159:VAL:HG22	1:D:198:VAL:HG12	1.98	0.46
1:C:206:VAL:O	1:C:207:ARG:C	2.54	0.46
1:D:330:SER:OG	1:D:353:ARG:HD2	2.16	0.46
1:C:34:HIS:HB3	1:C:37:ILE:CG2	2.45	0.46
1:C:69:ASN:O	1:C:73:ILE:HG22	2.15	0.46
1:C:299:GLU:O	1:C:300:LEU:C	2.53	0.46
1:A:59:TYR:N	1:A:60:PRO:CD	2.79	0.46
1:A:113:SER:HB2	1:A:115:ASP:OD1	2.15	0.46
1:B:172:TYR:N	1:B:173:PRO:HD2	2.31	0.45
1:C:161:VAL:HG12	1:C:196:VAL:HA	1.98	0.45
1:A:11:LEU:CD2	1:A:51:HIS:CD2	2.99	0.45
1:A:153:ARG:O	1:A:153:ARG:HG2	2.16	0.45
1:A:198:VAL:CG1	1:A:202:ARG:CG	2.94	0.45
1:B:352:TRP:O	1:B:353:ARG:HB2	2.17	0.45
1:C:8:PHE:CE2	1:C:9:GLY:O	2.70	0.45
1:B:221:TYR:N	1:B:221:TYR:CD1	2.84	0.45
1:A:188:PHE:HA	1:A:310:ASN:O	2.16	0.45
1:C:129:ARG:HG2	1:D:147:ARG:NH2	2.32	0.45
1:C:221:TYR:HD1	1:C:221:TYR:N	2.15	0.45
1:B:221:TYR:N	1:B:221:TYR:HD1	2.14	0.45
1:C:130:ARG:NH2	1:D:344:CYS:SG	2.90	0.45
1:C:161:VAL:CG1	1:C:196:VAL:HG22	2.46	0.45
1:C:298:LEU:O	1:C:301:THR:HG23	2.16	0.45
1:B:35:GLU:O	1:B:39:ARG:HG3	2.17	0.45
1:D:42:HIS:NE2	1:D:185:THR:CG2	2.66	0.45
1:A:134:PHE:HA	1:A:135:GLY:HA2	1.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:HG13	1:C:195:VAL:HG22	1.98	0.45
1:B:3:VAL:HG11	1:B:203:ALA:HB2	1.99	0.45
1:B:328:PRO:CB	1:B:329:PRO:HD3	2.46	0.45
1:C:253:LEU:O	1:C:254:ALA:C	2.56	0.45
1:A:308:ILE:HA	1:A:308:ILE:HD13	1.64	0.44
1:B:3:VAL:CG1	1:B:203:ALA:HB2	2.47	0.44
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.71	0.44
1:C:114:LEU:O	1:C:118:ILE:HD12	2.16	0.44
1:C:277:HIS:O	1:C:278:PRO:O	2.35	0.44
1:D:262:ASP:O	1:D:263:ALA:C	2.54	0.44
1:A:12:PRO:HD2	1:A:51:HIS:HB3	1.98	0.44
1:B:352:TRP:O	1:B:353:ARG:CB	2.66	0.44
1:D:100:MET:HG2	1:D:129:ARG:O	2.18	0.44
1:D:166:GLU:HG3	1:D:312:SER:HB3	2.00	0.44
1:C:221:TYR:N	1:C:221:TYR:CD1	2.85	0.44
1:D:18:GLN:HE22	1:D:50:ARG:HE	1.65	0.44
1:D:168:CYS:O	1:D:171:THR:OG1	2.28	0.44
1:A:253:LEU:HD23	1:A:290:SER:OG	2.17	0.44
1:A:309:GLY:O	1:A:311:LEU:CD1	2.66	0.44
1:B:144:GLY:HA3	1:B:162:LEU:HD22	2.00	0.44
1:A:328:PRO:C	1:A:329:PRO:O	2.56	0.44
1:C:315:SER:O	1:C:318:HIS:N	2.51	0.44
1:A:147:ARG:HA	1:A:147:ARG:HD3	1.77	0.43
1:A:249:ILE:HG23	1:A:253:LEU:HD22	1.99	0.43
1:C:15:ARG:HD2	1:C:16:TYR:N	2.33	0.43
1:C:101:ILE:HG23	1:C:101:ILE:O	2.17	0.43
1:D:211:PRO:HB3	1:D:352:TRP:CE3	2.53	0.43
1:B:337:LEU:CB	1:B:347:LEU:CD2	2.95	0.43
1:D:72:PHE:HA	1:D:170:LEU:CD2	2.44	0.43
1:A:211:PRO:HG3	1:A:352:TRP:CE3	2.53	0.43
1:A:58:GLN:O	1:A:61:SER:OG	2.34	0.43
1:C:261:LEU:HD12	1:C:261:LEU:HA	1.78	0.43
1:D:111:VAL:HA	1:D:112:PRO:C	2.38	0.43
1:A:65:PHE:CG	1:A:236:GLY:HA2	2.52	0.43
1:C:247:ASN:OD1	1:C:247:ASN:N	2.51	0.43
1:B:12:PRO:HG2	1:B:51:HIS:HB3	1.99	0.43
1:B:329:PRO:HD2	1:B:332:SER:CB	2.44	0.43
1:D:221:TYR:HD1	1:D:221:TYR:N	2.16	0.43
1:A:137:GLY:HA3	1:A:341:PRO:HD2	2.01	0.43
1:C:147:ARG:HH12	1:D:129:ARG:NH2	2.15	0.43
1:B:21:ILE:O	1:B:25:PHE:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:HIS:CE1	1:B:310:ASN:HD21	2.36	0.43
1:D:246:THR:O	1:D:250:GLU:CG	2.67	0.43
1:B:7:VAL:HG11	1:B:321:ARG:HB2	2.00	0.43
1:C:99:ASP:O	1:C:128:VAL:HG23	2.19	0.43
1:B:77:VAL:O	1:B:81:VAL:HG13	2.18	0.43
1:B:328:PRO:CB	1:B:329:PRO:CD	2.96	0.43
1:D:112:PRO:HD2	1:D:117:ARG:NH2	2.34	0.43
1:D:221:TYR:N	1:D:221:TYR:CD1	2.86	0.43
1:D:271:ILE:HD11	1:D:274:TRP:CG	2.54	0.43
1:C:10:ALA:C	1:C:11:LEU:HG	2.39	0.43
1:C:336:MET:HB2	1:C:348:VAL:HB	2.01	0.43
1:A:245:LEU:O	1:A:246:THR:C	2.56	0.42
1:D:15:ARG:CG	1:D:15:ARG:NH2	2.80	0.42
1:D:169:SER:OG	1:D:190:ASP:OD2	2.37	0.42
1:C:135:GLY:CA	1:D:111:VAL:HG22	2.43	0.42
1:C:228:MET:HA	1:C:240:ARG:O	2.19	0.42
1:B:106:VAL:HG12	1:B:166:GLU:OE1	2.19	0.42
1:B:199:GLY:O	1:B:203:ALA:N	2.50	0.42
1:D:172:TYR:N	1:D:173:PRO:CD	2.83	0.42
1:D:278:PRO:O	1:D:280:GLY:N	2.52	0.42
1:A:206:VAL:C	1:A:207:ARG:CG	2.85	0.42
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.84	0.42
1:A:115:ASP:OD1	1:A:132:PRO:HB3	2.19	0.42
1:C:149:ARG:O	1:C:153:ARG:HB2	2.19	0.42
1:B:95:PRO:HB3	1:B:124:LEU:HD23	2.01	0.42
1:A:84:LEU:HD22	1:A:88:LEU:HD22	2.01	0.42
1:D:352:TRP:HA	1:D:352:TRP:HE3	1.82	0.42
1:C:323:THR:O	1:C:326:LYS:HB2	2.20	0.42
1:B:228:MET:O	1:B:240:ARG:NH1	2.53	0.42
1:C:276:SER:HB3	1:C:301:THR:HG21	2.01	0.42
1:C:316:ILE:HG23	1:C:317:LEU:N	2.35	0.42
1:A:257:VAL:HG11	1:A:291:LEU:HD11	2.02	0.41
1:B:215:ASP:OD2	1:B:264:HIS:CE1	2.72	0.41
1:C:323:THR:O	1:C:326:LYS:CB	2.68	0.41
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.88	0.41
1:B:141:GLY:HA3	1:B:316:ILE:CG2	2.51	0.41
1:B:257:VAL:HG22	1:B:347:LEU:HD11	2.01	0.41
1:D:224:SER:HB2	1:D:227:ILE:HG13	2.02	0.41
1:B:264:HIS:O	1:B:266:LEU:HG	2.20	0.41
1:D:274:TRP:CD1	1:D:293:LEU:HD22	2.54	0.41
1:A:139:VAL:HG23	1:A:339:MET:CA	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HB	1:A:212:ASP:HA	2.03	0.41
1:A:324:ILE:HG22	1:A:325:GLU:N	2.34	0.41
1:B:7:VAL:HG22	1:B:195:VAL:HG13	2.03	0.41
1:A:47:VAL:HG22	1:A:305:LEU:O	2.21	0.41
1:A:228:MET:HE3	1:A:343:PHE:CE1	2.56	0.41
1:C:81:VAL:HG12	1:C:82:GLU:N	2.34	0.41
1:C:242:SER:HA	1:C:243:PRO:HD2	1.87	0.41
1:B:111:VAL:HA	1:B:112:PRO:C	2.40	0.41
1:B:201:ARG:HD3	1:D:353:ARG:CG	2.51	0.41
1:D:147:ARG:HA	1:D:147:ARG:NE	2.36	0.41
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.78	0.41
1:B:242:SER:OG	1:B:244:ASP:OD2	2.31	0.41
1:D:311:LEU:O	1:D:312:SER:HB3	2.21	0.41
1:A:198:VAL:CG1	1:A:202:ARG:HG2	2.50	0.41
1:C:37:ILE:CD1	1:C:40:ARG:NH2	2.61	0.41
1:C:162:LEU:O	1:C:194:ALA:HA	2.21	0.41
1:B:88:LEU:HD21	1:B:98:ILE:HD11	2.03	0.41
1:D:67:ASP:O	1:D:71:ILE:HG13	2.21	0.41
1:D:115:ASP:OD2	1:D:132:PRO:HB3	2.20	0.41
1:B:101:ILE:HG13	1:B:161:VAL:HG23	2.02	0.41
1:D:246:THR:HG23	1:D:247:ASN:N	2.36	0.41
1:A:81:VAL:O	1:A:82:GLU:C	2.58	0.40
1:C:135:GLY:HA2	1:D:111:VAL:CG2	2.43	0.40
1:B:106:VAL:HG11	1:B:137:GLY:HA2	2.03	0.40
1:B:294:PRO:HG2	1:B:296:GLU:HG2	2.03	0.40
1:D:46:LYS:HB2	1:D:281:PRO:HG3	2.03	0.40
1:A:131:MET:HG2	1:A:133:LEU:HD21	2.03	0.40
1:B:161:VAL:HG12	1:B:196:VAL:HG22	2.02	0.40
1:B:211:PRO:HB2	1:B:351:ARG:O	2.21	0.40
1:B:276:SER:HB3	1:B:301:THR:HG21	2.02	0.40
1:B:69:ASN:HD21	1:B:109:VAL:N	2.14	0.40
1:C:64:ASP:HB3	1:C:67:ASP:HB2	2.03	0.40
1:C:284:ILE:HA	1:C:287:VAL:CG1	2.52	0.40
1:C:314:ALA:O	1:C:317:LEU:HB2	2.22	0.40
1:B:1:MET:H2	1:B:149:ARG:HG2	1.86	0.40
1:B:211:PRO:CB	1:B:351:ARG:O	2.70	0.40
1:D:283:VAL:O	1:D:287:VAL:HG23	2.22	0.40
1:D:328:PRO:HB2	1:D:329:PRO:HD2	2.02	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:C:299:GLU:OE1	1:D:303:ARG:NH1[1_455]	2.07	0.13

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	350/353 (99%)	319 (91%)	27 (8%)	4 (1%)	14	5
1	B	351/353 (99%)	320 (91%)	25 (7%)	6 (2%)	9	2
1	C	350/353 (99%)	304 (87%)	38 (11%)	8 (2%)	6	1
1	D	350/353 (99%)	322 (92%)	21 (6%)	7 (2%)	7	1
All	All	1401/1412 (99%)	1265 (90%)	111 (8%)	25 (2%)	8	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	278	PRO
1	B	330	SER
1	D	205	GLN
1	D	206	VAL
1	D	352	TRP
1	A	329	PRO
1	C	299	GLU
1	C	300	LEU
1	B	329	PRO
1	D	292	ALA
1	A	205	GLN
1	B	328	PRO
1	B	332	SER
1	D	263	ALA
1	C	29	PRO
1	C	312	SER
1	B	263	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	327	ARG
1	A	245	LEU
1	A	327	ARG
1	D	327	ARG
1	C	341	PRO
1	D	106	VAL
1	C	81	VAL
1	C	106	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	280/281 (100%)	223 (80%)	57 (20%)	1	0
1	B	281/281 (100%)	236 (84%)	45 (16%)	2	0
1	C	280/281 (100%)	226 (81%)	54 (19%)	1	0
1	D	280/281 (100%)	234 (84%)	46 (16%)	2	0
All	All	1121/1124 (100%)	919 (82%)	202 (18%)	1	0

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	11	LEU
1	A	23	ASP
1	A	35	GLU
1	A	37	ILE
1	A	41	LEU
1	A	57	GLN
1	A	62	LEU
1	A	79	LEU
1	A	84	LEU
1	A	88	LEU
1	A	89	ASP
1	A	94	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	103	THR
1	A	109	VAL
1	A	115	ASP
1	A	138	CYS
1	A	139	VAL
1	A	148	LEU
1	A	161	VAL
1	A	162	LEU
1	A	164	SER
1	A	176	LYS
1	A	181	SER
1	A	185	THR
1	A	201	ARG
1	A	207	ARG
1	A	216	SER
1	A	220	LEU
1	A	223	ASP
1	A	225	LEU
1	A	230	TRP
1	A	231	ASP
1	A	237	LEU
1	A	241	LEU
1	A	246	THR
1	A	251	ARG
1	A	257	VAL
1	A	261	LEU
1	A	265	ARG
1	A	298	LEU
1	A	301	THR
1	A	303	ARG
1	A	305	LEU
1	A	308	ILE
1	A	310	ASN
1	A	313	SER
1	A	324	ILE
1	A	325	GLU
1	A	326	LYS
1	A	327	ARG
1	A	332	SER
1	A	339	MET
1	A	345	THR
1	A	347	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	LEU
1	A	353	ARG
1	C	15	ARG
1	C	19	SER
1	C	36	GLU
1	C	37	ILE
1	C	40	ARG
1	C	73	ILE
1	C	82	GLU
1	C	88	LEU
1	C	100	MET
1	C	103	THR
1	C	107	THR
1	C	114	LEU
1	C	115	ASP
1	C	124	LEU
1	C	129	ARG
1	C	134	PHE
1	C	136	LEU
1	C	147	ARG
1	C	148	LEU
1	C	157	ASP
1	C	170	LEU
1	C	176	LYS
1	C	178	THR
1	C	180	SER
1	C	185	THR
1	C	200	ASP
1	C	202	ARG
1	C	206	VAL
1	C	220	LEU
1	C	221	TYR
1	C	224	SER
1	C	237	LEU
1	C	245	LEU
1	C	247	ASN
1	C	250	GLU
1	C	251	ARG
1	C	252	TYR
1	C	255	ASN
1	C	258	THR
1	C	261	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	265	ARG
1	C	287	VAL
1	C	295	PRO
1	C	299	GLU
1	C	301	THR
1	C	305	LEU
1	C	307	GLU
1	C	326	LYS
1	C	327	ARG
1	C	329	PRO
1	C	339	MET
1	C	347	LEU
1	C	351	ARG
1	C	353	ARG
1	B	1	MET
1	B	11	LEU
1	B	15	ARG
1	B	17	SER
1	B	19	SER
1	B	41	LEU
1	B	81	VAL
1	B	96	SER
1	B	100	MET
1	B	107	THR
1	B	109	VAL
1	B	114	LEU
1	B	148	LEU
1	B	180	SER
1	B	181	SER
1	B	204	GLU
1	B	205	GLN
1	B	206	VAL
1	B	218	SER
1	B	221	TYR
1	B	239	LEU
1	B	241	LEU
1	B	244	ASP
1	B	246	THR
1	B	255	ASN
1	B	259	THR
1	B	265	ARG
1	B	267	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	268	LYS
1	B	287	VAL
1	B	293	LEU
1	B	294	PRO
1	B	296	GLU
1	B	300	LEU
1	B	301	THR
1	B	310	ASN
1	B	323	THR
1	B	326	LYS
1	B	327	ARG
1	B	330	SER
1	B	332	SER
1	B	337	LEU
1	B	339	MET
1	B	345	THR
1	B	353	ARG
1	D	15	ARG
1	D	18	GLN
1	D	31	LEU
1	D	33	GLU
1	D	37	ILE
1	D	39	ARG
1	D	40	ARG
1	D	54	LEU
1	D	56	LEU
1	D	58	GLN
1	D	84	LEU
1	D	88	LEU
1	D	89	ASP
1	D	92	ASN
1	D	103	THR
1	D	114	LEU
1	D	170	LEU
1	D	178	THR
1	D	201	ARG
1	D	202	ARG
1	D	206	VAL
1	D	207	ARG
1	D	212	ASP
1	D	221	TYR
1	D	234	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	237	LEU
1	D	245	LEU
1	D	248	LEU
1	D	250	GLU
1	D	251	ARG
1	D	256	ASP
1	D	262	ASP
1	D	267	THR
1	D	268	LYS
1	D	271	ILE
1	D	276	SER
1	D	290	SER
1	D	293	LEU
1	D	298	LEU
1	D	300	LEU
1	D	301	THR
1	D	310	ASN
1	D	326	LYS
1	D	350	LEU
1	D	351	ARG
1	D	353	ARG

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

Mol	Chain	Res	Type
1	A	51	HIS
1	A	69	ASN
1	A	310	ASN
1	C	48	ASN
1	C	205	GLN
1	C	318	HIS
1	B	51	HIS
1	B	69	ASN
1	B	205	GLN
1	B	247	ASN
1	B	255	ASN
1	B	264	HIS
1	B	310	ASN
1	D	18	GLN
1	D	92	ASN
1	D	310	ASN
1	D	318	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	352/353 (99%)	0.76	32 (9%) 9 10	24, 63, 79, 96	0
1	B	353/353 (100%)	0.80	46 (13%) 3 3	24, 61, 81, 94	0
1	C	352/353 (99%)	0.71	41 (11%) 4 5	22, 59, 83, 92	0
1	D	352/353 (99%)	0.80	40 (11%) 5 5	24, 63, 87, 96	0
All	All	1409/1412 (99%)	0.77	159 (11%) 5 5	22, 62, 83, 96	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.8
1	B	133	LEU	4.7
1	D	271	ILE	4.6
1	C	104	ALA	4.3
1	D	294	PRO	4.3
1	B	134	PHE	4.2
1	C	353	ARG	4.2
1	A	134	PHE	4.2
1	C	132	PRO	4.1
1	A	133	LEU	4.0
1	D	133	LEU	4.0
1	A	102	ALA	4.0
1	C	133	LEU	3.9
1	B	104	ALA	3.9
1	B	143	ALA	3.9
1	A	103	THR	3.8
1	B	139	VAL	3.8
1	A	132	PRO	3.8
1	A	28	PHE	3.7
1	A	101	ILE	3.6
1	A	143	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	102	ALA	3.6
1	B	137	GLY	3.6
1	B	266	LEU	3.5
1	D	132	PRO	3.4
1	B	135	GLY	3.4
1	B	132	PRO	3.4
1	A	105	THR	3.4
1	C	206	VAL	3.4
1	A	163	VAL	3.4
1	D	137	GLY	3.3
1	A	114	LEU	3.3
1	D	353	ARG	3.3
1	B	140	ALA	3.3
1	A	353	ARG	3.3
1	B	245	LEU	3.2
1	D	146	ALA	3.2
1	B	105	THR	3.2
1	D	134	PHE	3.2
1	B	109	VAL	3.2
1	D	104	ALA	3.1
1	A	93	LEU	3.1
1	A	165	VAL	3.1
1	B	265	ARG	3.1
1	A	104	ALA	3.1
1	C	131	MET	3.1
1	A	31	LEU	3.0
1	A	131	MET	3.0
1	D	292	ALA	3.0
1	C	134	PHE	3.0
1	C	103	THR	3.0
1	C	114	LEU	3.0
1	A	110	ALA	3.0
1	A	137	GLY	2.9
1	B	316	ILE	2.9
1	A	111	VAL	2.9
1	B	348	VAL	2.9
1	C	208	ALA	2.9
1	C	93	LEU	2.9
1	D	114	LEU	2.9
1	C	143	ALA	2.9
1	A	139	VAL	2.8
1	B	102	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	142	ALA	2.8
1	D	102	ALA	2.8
1	C	139	VAL	2.8
1	B	142	ALA	2.7
1	B	257	VAL	2.7
1	B	207	ARG	2.7
1	B	267	THR	2.7
1	C	111	VAL	2.7
1	B	106	VAL	2.7
1	A	144	GLY	2.6
1	B	145	VAL	2.6
1	B	85	LEU	2.6
1	C	254	ALA	2.6
1	A	145	VAL	2.6
1	D	142	ALA	2.6
1	D	139	VAL	2.6
1	C	135	GLY	2.6
1	A	106	VAL	2.6
1	C	145	VAL	2.6
1	C	162	LEU	2.6
1	D	141	GLY	2.6
1	A	146	ALA	2.5
1	B	276	SER	2.5
1	C	314	ALA	2.5
1	B	144	GLY	2.5
1	C	246	THR	2.5
1	D	143	ALA	2.5
1	B	28	PHE	2.5
1	D	293	LEU	2.5
1	C	209	GLY	2.5
1	B	26	VAL	2.5
1	D	106	VAL	2.5
1	D	138	CYS	2.5
1	D	295	PRO	2.4
1	B	161	VAL	2.4
1	D	145	VAL	2.4
1	C	245	LEU	2.4
1	D	266	LEU	2.4
1	C	265	ARG	2.4
1	C	204	GLU	2.4
1	A	324	ILE	2.4
1	D	29	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	162	LEU	2.4
1	C	317	LEU	2.4
1	B	138	CYS	2.4
1	C	249	ILE	2.4
1	C	235	HIS	2.3
1	D	148	LEU	2.3
1	A	141	GLY	2.3
1	D	103	THR	2.3
1	B	165	VAL	2.3
1	C	344	CYS	2.3
1	A	32	LYS	2.3
1	C	348	VAL	2.3
1	B	131	MET	2.3
1	C	140	ALA	2.3
1	D	311	LEU	2.3
1	B	353	ARG	2.3
1	D	352	TRP	2.3
1	B	347	LEU	2.3
1	D	131	MET	2.2
1	A	109	VAL	2.2
1	D	101	ILE	2.2
1	C	141	GLY	2.2
1	D	144	GLY	2.2
1	D	130	ARG	2.2
1	B	108	GLY	2.2
1	C	148	LEU	2.2
1	C	106	VAL	2.2
1	B	319	ILE	2.2
1	D	89	ASP	2.2
1	D	165	VAL	2.2
1	C	330	SER	2.2
1	B	208	ALA	2.2
1	B	344	CYS	2.2
1	C	320	LEU	2.1
1	D	246	THR	2.1
1	B	113	SER	2.1
1	C	290	SER	2.1
1	B	230	TRP	2.1
1	C	116	ALA	2.1
1	D	291	LEU	2.1
1	B	221	TYR	2.1
1	D	267	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	338	ALA	2.1
1	D	31	LEU	2.1
1	D	84	LEU	2.1
1	C	144	GLY	2.1
1	A	14	HIS	2.0
1	C	101	ILE	2.0
1	D	317	LEU	2.0
1	B	313	SER	2.0
1	B	206	VAL	2.0
1	D	147	ARG	2.0
1	B	337	LEU	2.0
1	B	349	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.