



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:54 am GMT

PDB ID : 2E32
Title : Structural basis for selection of glycosylated substrate by SCFFbs1 ubiquitin ligase
Authors : Mizushima, T.; Yoshida, Y.; Kumanomidou, T.; Hasegawa, Y.; Yamane, T.; Tanaka, K.
Deposited on : 2006-11-20
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

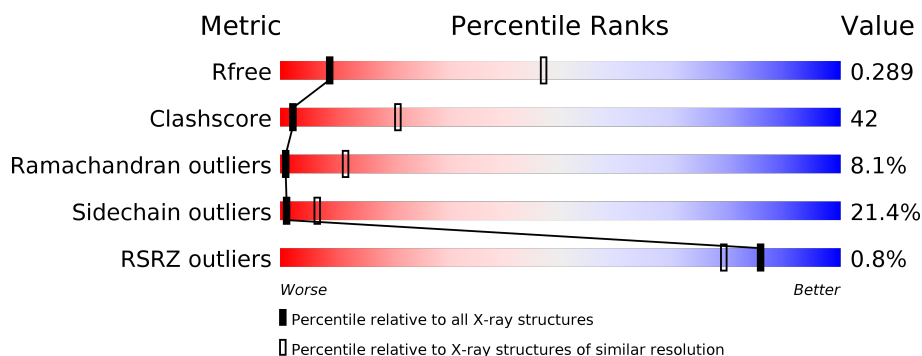
1 Overall quality at a glance

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}	100719	1239 (3.64-3.40)
Clashscore	112137	1007 (3.62-3.42)
Ramachandran outliers	110173	1328 (3.64-3.40)
Sidechain outliers	110143	1329 (3.64-3.40)
RSRZ outliers	101464	1270 (3.64-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	297	<div> <div> <div>1%</div> <div>30%</div> <div>37%</div> <div>12%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	297	<div> <div>31%</div> <div>37%</div> <div>11%</div> <div>•</div> <div>19%</div> </div>
2	B	166	<div> <div>2%</div> <div>17%</div> <div>44%</div> <div>15%</div> <div>•</div> <div>22%</div> </div>
2	D	166	<div> <div>14%</div> <div>46%</div> <div>16%</div> <div>•</div> <div>22%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5970 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 F-box only protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1948	1249	324	369	6			
1	C	240	Total	C	N	O	S	0	0	0
			1948	1249	324	369	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LYS	ARG	SEE REMARK 999	UNP Q80UW2
C	151	LYS	ARG	SEE REMARK 999	UNP Q80UW2

- Molecule 2 is a protein called S-phase kinase-associated protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			1037	660	167	206	4			
2	D	130	Total	C	N	O	S	0	0	0
			1037	660	167	206	4			

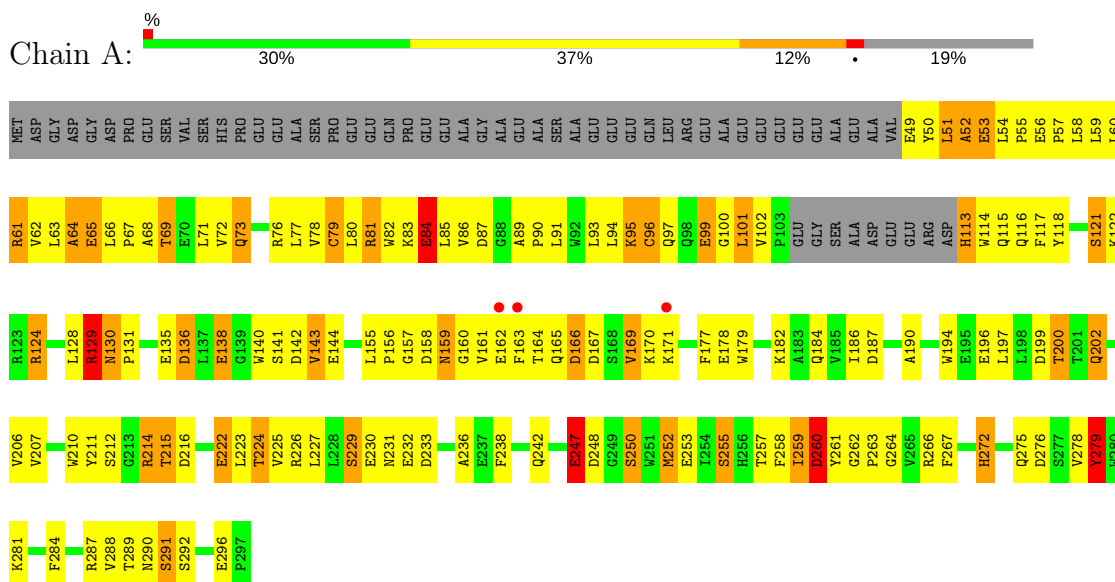
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	CLONING ARTIFACT	UNP P63208
B	-1	PRO	-	CLONING ARTIFACT	UNP P63208
B	0	HIS	-	CLONING ARTIFACT	UNP P63208
D	-2	GLY	-	CLONING ARTIFACT	UNP P63208
D	-1	PRO	-	CLONING ARTIFACT	UNP P63208
D	0	HIS	-	CLONING ARTIFACT	UNP P63208

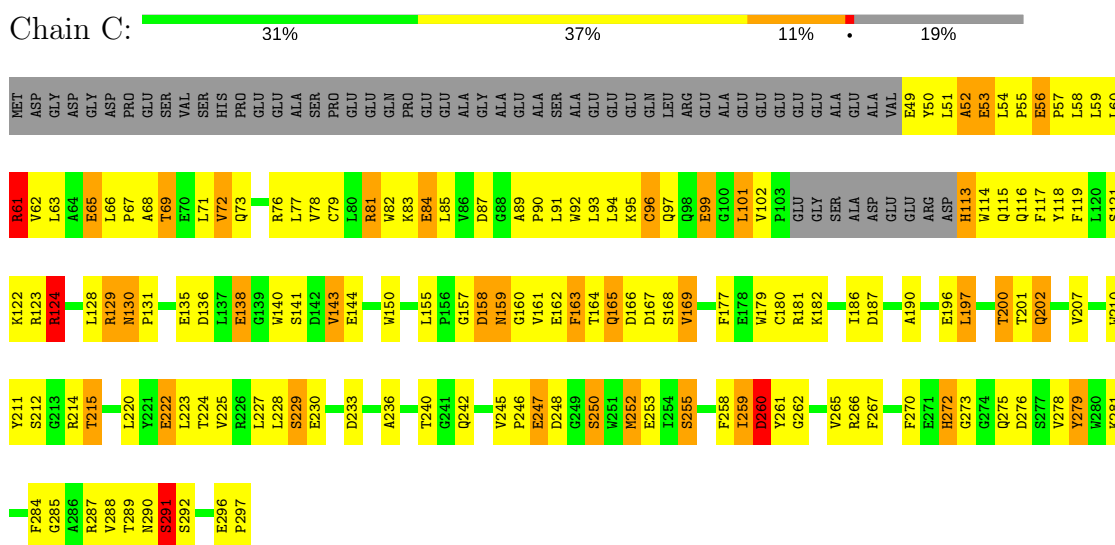
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

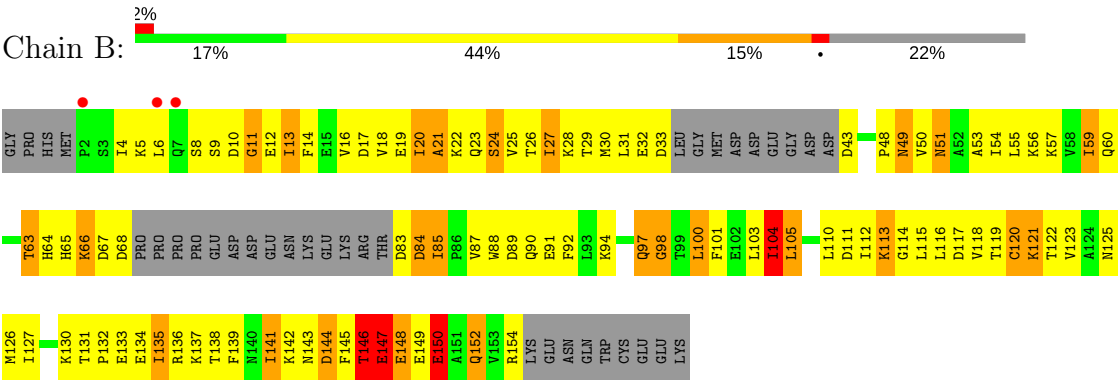
• Molecule 1: F-box only protein 2



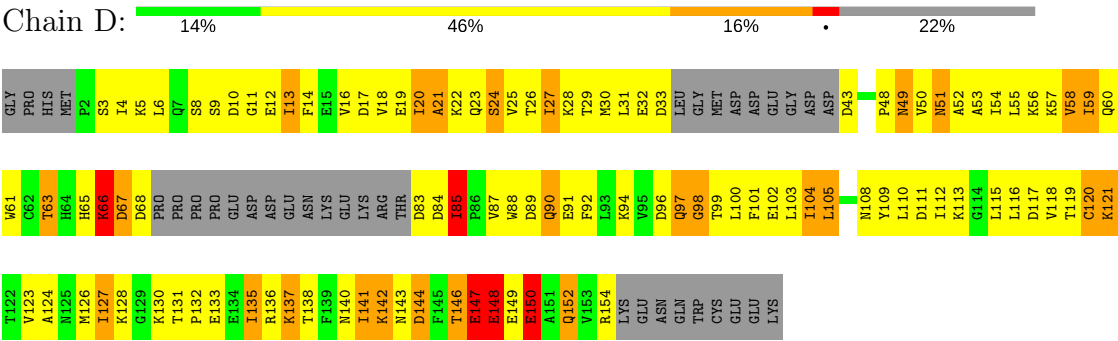
• Molecule 1: F-box only protein 2



• Molecule 2: S-phase kinase-associated protein 1A



● Molecule 2: S-phase kinase-associated protein 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.94Å 109.82Å 153.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.53 – 3.52 56.53 – 3.52	Depositor EDS
% Data completeness (in resolution range)	89.7 (56.53-3.52) 89.7 (56.53-3.52)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.223 , 0.299 0.218 , 0.289	Depositor DCC
R_{free} test set	650 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5970	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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	1.06	2/2003 (0.1%)	1.00	2/2725 (0.1%)
1	C	1.01	1/2003 (0.0%)	0.97	1/2725 (0.0%)
2	B	1.13	5/1052 (0.5%)	1.11	3/1422 (0.2%)
2	D	1.10	3/1052 (0.3%)	1.09	2/1422 (0.1%)
All	All	1.06	11/6110 (0.2%)	1.02	8/8294 (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	C	0	1
2	B	0	2
2	D	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	113	LYS	CD-CE	8.71	1.73	1.51
2	D	113	LYS	CD-CE	8.16	1.71	1.51
1	A	296	GLU	CG-CD	7.51	1.63	1.51
1	A	279	TYR	CE2-CZ	6.92	1.47	1.38
2	D	150	GLU	CB-CG	6.13	1.63	1.52
2	B	133	GLU	CG-CD	5.80	1.60	1.51
2	D	113	LYS	CG-CD	5.78	1.72	1.52
2	B	120	CYS	CB-SG	-5.67	1.72	1.81
1	C	92	TRP	CB-CG	-5.51	1.40	1.50
2	B	113	LYS	CG-CD	5.35	1.70	1.52
2	B	150	GLU	CB-CG	5.12	1.61	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	129	ARG	NE-CZ-NH1	5.93	123.26	120.30
2	D	113	LYS	CB-CG-CD	5.85	126.81	111.60
2	B	113	LYS	CB-CG-CD	5.77	126.61	111.60
1	A	226	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	D	113	LYS	CB-CA-C	5.15	120.70	110.40
2	B	11	GLY	N-CA-C	5.11	125.88	113.10
2	B	113	LYS	CB-CA-C	5.07	120.53	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	146	THR	Peptide
2	B	83	ASP	Peptide
1	C	165	GLN	Peptide
2	D	83	ASP	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	1948	0	1847	139	1
1	C	1948	0	1847	128	0
2	B	1037	0	1041	123	1
2	D	1037	0	1041	123	0
All	All	5970	0	5776	497	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 42.

All (497) 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)
2:D:148:GLU:O	2:D:149:GLU:HG3	1.41	1.19
2:B:64:HIS:CE1	2:D:128:LYS:HE2	1.81	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:HIS:HE1	2:D:128:LYS:HE2	1.05	1.15
2:B:148:GLU:O	2:B:149:GLU:HG3	1.57	1.03
2:B:64:HIS:HE1	2:D:128:LYS:CE	1.72	1.01
2:B:116:LEU:O	2:B:119:THR:HG22	1.61	0.99
1:A:212:SER:O	1:A:287:ARG:HG2	1.66	0.95
2:D:26:THR:HG23	2:D:111:ASP:HB2	1.48	0.94
1:C:138:GLU:OE2	1:C:138:GLU:HA	1.68	0.93
2:D:116:LEU:O	2:D:119:THR:HG22	1.69	0.92
1:A:138:GLU:OE2	1:A:138:GLU:HA	1.66	0.92
2:D:51:ASN:HD22	2:D:53:ALA:H	1.19	0.91
2:B:51:ASN:HD22	2:B:53:ALA:H	1.18	0.91
2:B:115:LEU:O	2:B:115:LEU:HD23	1.72	0.90
2:B:26:THR:HG23	2:B:111:ASP:HB2	1.53	0.90
2:B:26:THR:HG23	2:B:111:ASP:CB	2.03	0.89
1:A:61:ARG:HH11	1:A:61:ARG:HB3	1.37	0.89
2:B:117:ASP:OD2	2:B:121:LYS:HE2	1.74	0.87
1:A:89:ALA:N	1:A:90:PRO:HD2	1.90	0.85
1:A:135:GLU:HB2	1:A:138:GLU:HB2	1.59	0.84
1:C:135:GLU:HB2	1:C:138:GLU:HB2	1.58	0.84
1:A:68:ALA:O	1:A:72:VAL:HG23	1.77	0.83
1:C:163:PHE:CD2	1:C:169:VAL:HG21	2.14	0.82
2:D:97:GLN:HG2	2:D:101:PHE:HE1	1.45	0.81
2:D:135:ILE:HG13	2:D:136:ARG:N	1.95	0.81
1:C:227:LEU:HD12	1:C:236:ALA:HB3	1.60	0.81
2:D:21:ALA:C	2:D:23:GLN:H	1.82	0.81
1:C:140:TRP:CD2	1:C:182:LYS:HD2	2.16	0.81
1:C:61:ARG:HB3	1:C:61:ARG:HH11	1.43	0.81
1:C:89:ALA:N	1:C:90:PRO:HD2	1.95	0.81
1:C:54:LEU:HD12	1:C:55:PRO:HD2	1.62	0.80
1:C:212:SER:O	1:C:287:ARG:HG2	1.82	0.80
2:D:26:THR:HG23	2:D:111:ASP:CB	2.12	0.79
2:D:104:ILE:HB	2:D:119:THR:CG2	2.12	0.78
2:B:136:ARG:HG2	2:B:141:ILE:O	1.83	0.78
2:D:97:GLN:HG2	2:D:101:PHE:CE1	2.19	0.77
2:D:26:THR:CG2	2:D:111:ASP:HB2	2.15	0.76
2:B:101:PHE:HA	2:B:104:ILE:HG23	1.68	0.76
1:C:65:GLU:OE2	1:C:65:GLU:HA	1.86	0.75
2:B:21:ALA:C	2:B:23:GLN:H	1.88	0.75
1:C:141:SER:C	1:C:143:VAL:H	1.89	0.75
1:A:52:ALA:HB1	1:A:81:ARG:HH12	1.53	0.74
1:C:196:GLU:O	1:C:200:THR:HB	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASP:O	2:B:85:ILE:HG12	1.87	0.73
2:B:24:SER:OG	2:B:27:ILE:HG23	1.88	0.73
2:D:123:VAL:O	2:D:126:MET:HB2	1.88	0.72
2:D:32:GLU:O	2:D:33:ASP:HB2	1.89	0.72
2:B:26:THR:CG2	2:B:111:ASP:HB2	2.20	0.71
1:A:182:LYS:NZ	1:A:272:HIS:NE2	2.36	0.71
2:D:104:ILE:HB	2:D:119:THR:HG21	1.71	0.71
2:D:115:LEU:O	2:D:115:LEU:HD23	1.90	0.71
1:A:159:ASN:HD22	1:A:159:ASN:C	1.94	0.70
2:D:136:ARG:HG2	2:D:141:ILE:O	1.92	0.70
1:C:78:VAL:O	2:D:136:ARG:NH1	2.24	0.70
2:B:57:LYS:HG3	2:B:92:PHE:CZ	2.27	0.69
1:C:78:VAL:HG11	2:D:135:ILE:HD11	1.73	0.69
1:A:96:CYS:HA	1:A:101:LEU:HD12	1.74	0.69
1:A:54:LEU:HD12	1:A:55:PRO:HD2	1.74	0.69
2:D:57:LYS:HG3	2:D:92:PHE:CZ	2.27	0.69
2:D:10:ASP:O	2:D:12:GLU:N	2.24	0.69
1:A:210:TRP:CE3	1:A:253:GLU:HB2	2.28	0.69
1:A:247:GLU:HG2	1:A:248:ASP:H	1.58	0.69
1:A:89:ALA:H	1:A:90:PRO:HD2	1.55	0.69
2:B:56:LYS:HG3	2:B:60:GLN:HE21	1.58	0.68
2:B:91:GLU:O	2:B:94:LYS:HB2	1.93	0.68
2:D:63:THR:O	2:D:66:LYS:HG3	1.93	0.68
2:B:147:GLU:OE2	2:B:148:GLU:O	2.11	0.68
2:B:22:LYS:HG3	2:B:28:LYS:HG3	1.75	0.68
2:D:131:THR:O	2:D:135:ILE:HG23	1.93	0.68
2:B:10:ASP:O	2:B:12:GLU:N	2.26	0.68
2:D:22:LYS:HG3	2:D:28:LYS:HG3	1.75	0.68
2:B:115:LEU:C	2:B:115:LEU:HD23	2.13	0.68
2:B:63:THR:O	2:B:66:LYS:HG3	1.94	0.68
2:B:122:THR:O	2:B:125:ASN:HB2	1.92	0.68
1:A:141:SER:C	1:A:143:VAL:H	1.96	0.67
1:A:58:LEU:N	1:A:58:LEU:HD23	2.09	0.67
2:D:136:ARG:HA	2:D:141:ILE:HG23	1.75	0.67
1:A:186:ILE:O	1:A:267:PHE:HA	1.94	0.67
2:B:147:GLU:OE2	2:B:148:GLU:C	2.33	0.67
1:A:206:VAL:HG22	1:A:257:THR:HG23	1.75	0.67
1:C:227:LEU:HD11	1:C:258:PHE:CD1	2.30	0.67
2:D:57:LYS:HG3	2:D:92:PHE:CE1	2.29	0.67
1:A:227:LEU:HD12	1:A:236:ALA:HB3	1.77	0.66
1:A:101:LEU:HD22	1:A:121:SER:HB3	1.75	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:GLU:O	2:D:33:ASP:CB	2.43	0.66
1:C:207:VAL:O	1:C:255:SER:HA	1.94	0.66
1:C:187:ASP:HB3	1:C:190:ALA:HB3	1.77	0.66
1:C:247:GLU:HG2	1:C:248:ASP:H	1.59	0.66
2:B:97:GLN:HG2	2:B:101:PHE:HE1	1.61	0.66
2:B:54:ILE:O	2:B:55:LEU:C	2.33	0.65
1:A:52:ALA:HB1	1:A:81:ARG:NH1	2.10	0.65
1:A:52:ALA:CB	1:A:81:ARG:HH12	2.09	0.65
1:C:210:TRP:CE3	1:C:253:GLU:HB2	2.31	0.65
2:D:21:ALA:C	2:D:23:GLN:N	2.50	0.65
2:D:130:LYS:HB2	2:D:135:ILE:HG22	1.78	0.65
1:A:210:TRP:CE2	1:A:253:GLU:HG3	2.33	0.64
1:A:135:GLU:HB2	1:A:138:GLU:CB	2.28	0.64
2:B:103:LEU:C	2:B:105:LEU:H	1.99	0.64
2:B:26:THR:HG23	2:B:111:ASP:HB3	1.79	0.64
2:D:101:PHE:HA	2:D:104:ILE:HG23	1.78	0.64
1:A:51:LEU:O	1:A:53:GLU:N	2.30	0.64
1:C:182:LYS:NZ	1:C:272:HIS:NE2	2.40	0.64
2:D:27:ILE:C	2:D:27:ILE:HD12	2.18	0.64
2:B:116:LEU:O	2:B:119:THR:CG2	2.43	0.63
1:C:229:SER:HB3	1:C:233:ASP:HB2	1.80	0.63
1:A:289:THR:O	1:A:290:ASN:HB3	1.99	0.63
1:A:113:HIS:CE1	1:A:115:GLN:HB3	2.34	0.62
2:B:103:LEU:O	2:B:105:LEU:N	2.32	0.62
1:C:101:LEU:HD22	1:C:121:SER:HB3	1.80	0.62
1:A:78:VAL:O	2:B:136:ARG:NH1	2.33	0.62
1:C:62:VAL:O	1:C:65:GLU:HB2	1.99	0.62
2:D:104:ILE:HB	2:D:119:THR:HG23	1.80	0.62
1:C:68:ALA:O	1:C:72:VAL:HG23	2.00	0.61
1:C:155:LEU:CD1	1:C:163:PHE:HB2	2.30	0.61
2:B:97:GLN:HG2	2:B:101:PHE:CE1	2.35	0.61
2:B:26:THR:OG1	2:B:110:LEU:HA	2.01	0.61
1:A:212:SER:HB2	1:A:250:SER:O	2.01	0.61
1:C:89:ALA:H	1:C:90:PRO:HD2	1.64	0.61
2:D:126:MET:O	2:D:130:LYS:HE2	2.00	0.61
1:A:229:SER:HB3	1:A:233:ASP:HB2	1.82	0.61
2:D:21:ALA:O	2:D:23:GLN:N	2.34	0.61
1:C:57:PRO:HA	1:C:60:LEU:HD23	1.82	0.61
1:C:210:TRP:CD1	1:C:290:ASN:ND2	2.67	0.61
1:C:247:GLU:HG2	1:C:248:ASP:N	2.16	0.61
2:D:22:LYS:CG	2:D:28:LYS:HG3	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:GLU:OE1	2:D:150:GLU:N	2.34	0.60
2:B:51:ASN:ND2	2:B:53:ALA:HB3	2.16	0.60
2:D:148:GLU:O	2:D:149:GLU:CG	2.34	0.60
1:C:96:CYS:HA	1:C:101:LEU:HD12	1.82	0.60
2:B:148:GLU:OE1	2:B:150:GLU:N	2.35	0.60
1:C:135:GLU:HB2	1:C:138:GLU:CB	2.30	0.60
1:A:140:TRP:CD2	1:A:182:LYS:HD2	2.36	0.60
1:A:89:ALA:N	1:A:90:PRO:CD	2.65	0.60
2:D:51:ASN:HD21	2:D:53:ALA:HB3	1.66	0.60
1:C:163:PHE:HD2	1:C:166:ASP:O	1.83	0.60
2:D:17:ASP:O	2:D:20:ILE:HD13	2.01	0.60
2:D:87:VAL:O	2:D:90:GLN:HB2	2.02	0.60
1:A:135:GLU:CB	1:A:138:GLU:HG2	2.31	0.60
1:C:288:VAL:O	1:C:289:THR:HB	2.01	0.60
2:B:104:ILE:HB	2:B:119:THR:CG2	2.33	0.59
1:C:210:TRP:CE2	1:C:253:GLU:HG3	2.37	0.59
1:C:223:LEU:HB3	1:C:240:THR:HG23	1.84	0.59
2:B:51:ASN:HD21	2:B:53:ALA:HB3	1.67	0.59
1:C:207:VAL:HG11	1:C:225:VAL:HG21	1.84	0.59
2:D:65:HIS:O	2:D:67:ASP:N	2.36	0.59
1:C:141:SER:C	1:C:143:VAL:N	2.56	0.59
1:C:61:ARG:HH11	1:C:61:ARG:CB	2.12	0.58
1:A:51:LEU:HD13	1:A:52:ALA:N	2.18	0.58
1:A:78:VAL:HG11	2:B:135:ILE:HD11	1.86	0.58
2:B:21:ALA:C	2:B:23:GLN:N	2.56	0.58
2:D:137:LYS:HD3	2:D:138:THR:HG23	1.84	0.58
1:A:210:TRP:CZ3	1:A:253:GLU:HB2	2.37	0.58
1:A:278:VAL:O	1:A:279:TYR:HB3	2.04	0.58
2:B:87:VAL:O	2:B:90:GLN:HB2	2.04	0.58
1:A:157:GLY:HA3	1:A:287:ARG:HH12	1.69	0.58
2:B:87:VAL:HG22	1:C:73:GLN:OE1	2.04	0.58
2:D:4:ILE:N	2:D:16:VAL:O	2.33	0.58
1:A:196:GLU:O	1:A:200:THR:HB	2.03	0.58
1:A:129:ARG:HB3	1:A:129:ARG:NH1	2.19	0.58
1:A:278:VAL:O	1:A:279:TYR:CB	2.51	0.58
2:D:26:THR:OG1	2:D:110:LEU:HA	2.04	0.58
1:A:222:GLU:HG2	1:A:223:LEU:N	2.18	0.57
2:D:51:ASN:ND2	2:D:53:ALA:H	1.96	0.57
2:D:97:GLN:CG	2:D:101:PHE:HE1	2.15	0.57
2:B:104:ILE:HB	2:B:119:THR:HG21	1.86	0.57
2:B:116:LEU:C	2:B:119:THR:HG22	2.24	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:HG2	1:A:248:ASP:N	2.19	0.57
2:B:89:ASP:O	2:B:90:GLN:C	2.43	0.56
2:B:57:LYS:HE3	2:B:92:PHE:CE1	2.40	0.56
2:B:97:GLN:O	2:B:98:GLY:C	2.44	0.56
1:A:163:PHE:CD2	1:A:169:VAL:HG21	2.39	0.56
1:C:113:HIS:CE1	1:C:115:GLN:HB3	2.41	0.56
1:A:50:TYR:HA	1:A:53:GLU:OE1	2.04	0.56
1:A:155:LEU:CD1	1:A:163:PHE:HB2	2.36	0.56
2:B:135:ILE:HG13	2:B:136:ARG:N	2.17	0.56
2:B:4:ILE:HG23	2:B:6:LEU:CD1	2.36	0.56
2:B:103:LEU:C	2:B:105:LEU:N	2.59	0.55
2:B:27:ILE:C	2:B:27:ILE:HD12	2.27	0.55
1:C:89:ALA:N	1:C:90:PRO:CD	2.69	0.55
1:A:63:LEU:O	1:A:65:GLU:N	2.39	0.55
2:D:65:HIS:C	2:D:67:ASP:H	2.09	0.55
2:D:24:SER:OG	2:D:27:ILE:HG23	2.06	0.55
2:B:119:THR:HG23	2:B:120:CYS:N	2.22	0.55
2:D:55:LEU:O	2:D:59:ILE:HG23	2.06	0.55
1:A:51:LEU:C	1:A:53:GLU:H	2.09	0.55
1:C:159:ASN:HD22	1:C:159:ASN:C	2.10	0.55
2:D:96:ASP:O	2:D:97:GLN:C	2.45	0.54
1:C:210:TRP:CZ3	1:C:253:GLU:HB2	2.41	0.54
2:B:10:ASP:CG	2:B:10:ASP:O	2.45	0.54
2:B:51:ASN:ND2	2:B:53:ALA:H	1.98	0.54
1:C:164:THR:O	1:C:166:ASP:N	2.40	0.54
1:C:81:ARG:HA	1:C:84:GLU:OE2	2.08	0.54
2:B:4:ILE:HD12	2:B:5:LYS:H	1.73	0.54
1:C:265:VAL:O	1:C:266:ARG:NH1	2.39	0.54
2:B:85:ILE:HB	2:B:118:VAL:HG23	1.90	0.54
1:A:131:PRO:HB3	1:A:291:SER:O	2.08	0.53
1:C:177:PHE:CD2	1:C:281:LYS:HA	2.43	0.53
2:D:97:GLN:O	2:D:98:GLY:C	2.45	0.53
1:A:281:LYS:O	1:A:284:PHE:HE2	1.92	0.53
2:B:57:LYS:HG3	2:B:92:PHE:CE1	2.43	0.53
1:C:123:ARG:O	1:C:124:ARG:C	2.47	0.53
2:D:4:ILE:HG23	2:D:6:LEU:CD1	2.38	0.53
2:B:136:ARG:HA	2:B:141:ILE:HG23	1.90	0.53
1:C:71:LEU:HD13	1:C:91:LEU:HD11	1.89	0.53
2:D:115:LEU:C	2:D:115:LEU:HD23	2.29	0.53
2:B:85:ILE:HG13	2:B:90:GLN:HG2	1.91	0.53
2:D:123:VAL:O	2:D:126:MET:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ILE:O	2:B:104:ILE:HG13	2.08	0.53
1:C:210:TRP:HD1	1:C:290:ASN:HD22	1.53	0.53
1:A:49:GLU:O	1:A:53:GLU:OE1	2.27	0.53
1:A:159:ASN:ND2	1:A:215:THR:OG1	2.42	0.52
1:A:207:VAL:O	1:A:255:SER:HA	2.09	0.52
1:A:68:ALA:O	1:A:69:THR:C	2.47	0.52
1:C:51:LEU:HD13	1:C:51:LEU:C	2.30	0.52
1:C:69:THR:O	1:C:73:GLN:HB2	2.10	0.52
2:B:4:ILE:HG23	2:B:6:LEU:HD13	1.90	0.52
2:B:130:LYS:HB2	2:B:135:ILE:HG22	1.90	0.52
1:C:259:ILE:O	1:C:260:ASP:C	2.48	0.52
1:A:141:SER:C	1:A:143:VAL:N	2.63	0.52
1:C:60:LEU:H	1:C:60:LEU:HD22	1.74	0.52
1:A:164:THR:O	1:A:166:ASP:N	2.38	0.52
2:D:149:GLU:O	2:D:150:GLU:C	2.47	0.52
2:D:16:VAL:HB	2:D:20:ILE:HD11	1.91	0.52
1:A:96:CYS:HA	1:A:101:LEU:CD1	2.40	0.52
2:B:49:ASN:HD22	2:B:49:ASN:N	2.07	0.52
2:D:89:ASP:O	2:D:90:GLN:C	2.48	0.52
1:A:214:ARG:HG2	1:A:216:ASP:OD2	2.09	0.52
1:A:80:LEU:HD22	2:B:145:PHE:CE1	2.45	0.52
2:B:17:ASP:OD1	2:B:19:GLU:HB3	2.09	0.52
2:D:117:ASP:OD2	2:D:121:LYS:HE2	2.09	0.52
2:D:84:ASP:O	2:D:85:ILE:HG12	2.10	0.52
2:D:88:TRP:O	2:D:91:GLU:HB3	2.10	0.51
1:A:138:GLU:OE2	1:A:138:GLU:CA	2.50	0.51
2:B:21:ALA:O	2:B:22:LYS:CB	2.58	0.51
2:B:54:ILE:O	2:B:57:LYS:N	2.43	0.51
1:A:135:GLU:HB3	1:A:138:GLU:HG2	1.93	0.51
2:B:115:LEU:C	2:B:115:LEU:CD2	2.77	0.51
1:C:58:LEU:HD23	1:C:58:LEU:N	2.26	0.51
1:C:49:GLU:HG2	2:D:140:ASN:HB3	1.93	0.51
2:D:57:LYS:O	2:D:60:GLN:HB2	2.11	0.51
2:B:137:LYS:HD3	2:B:138:THR:HG23	1.92	0.51
1:C:129:ARG:NH1	1:C:129:ARG:HB3	2.26	0.51
1:A:129:ARG:HB3	1:A:129:ARG:CZ	2.40	0.51
1:C:116:GLN:O	1:C:117:PHE:C	2.49	0.51
1:C:289:THR:O	1:C:290:ASN:HB3	2.11	0.51
2:D:147:GLU:OE2	2:D:149:GLU:HA	2.11	0.51
1:A:128:LEU:HD12	1:A:291:SER:C	2.31	0.51
2:B:126:MET:O	2:B:130:LYS:HE2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:LEU:C	2:D:105:LEU:H	2.13	0.51
2:B:123:VAL:O	2:B:126:MET:HB2	2.11	0.51
1:C:94:LEU:O	1:C:95:LYS:C	2.47	0.51
1:A:116:GLN:O	1:A:117:PHE:C	2.49	0.51
1:A:187:ASP:HB3	1:A:190:ALA:HB3	1.93	0.50
1:C:202:GLN:HE22	1:C:262:GLY:C	2.14	0.50
2:D:51:ASN:ND2	2:D:53:ALA:HB3	2.26	0.50
2:D:97:GLN:O	2:D:100:LEU:HB2	2.12	0.50
1:A:135:GLU:HB2	1:A:138:GLU:HG2	1.92	0.50
2:B:104:ILE:O	2:B:104:ILE:CG1	2.59	0.50
2:B:32:GLU:O	2:B:33:ASP:HB2	2.12	0.50
1:C:159:ASN:ND2	1:C:215:THR:OG1	2.45	0.50
1:C:259:ILE:O	1:C:261:TYR:N	2.44	0.50
1:C:281:LYS:O	1:C:284:PHE:HE2	1.95	0.50
2:D:103:LEU:C	2:D:105:LEU:N	2.64	0.50
2:D:10:ASP:CG	2:D:10:ASP:O	2.50	0.50
1:A:156:PRO:HB3	1:A:162:GLU:HB2	1.93	0.50
1:C:223:LEU:HD13	1:C:272:HIS:HB3	1.94	0.50
2:D:142:LYS:HD3	2:D:143:ASN:N	2.27	0.50
2:D:14:PHE:CD2	2:D:55:LEU:HD23	2.47	0.50
2:D:135:ILE:CG1	2:D:136:ARG:N	2.72	0.50
2:D:4:ILE:HG23	2:D:6:LEU:HD13	1.93	0.49
2:B:119:THR:O	2:B:122:THR:HB	2.11	0.49
1:C:212:SER:HB2	1:C:250:SER:O	2.13	0.49
1:C:211:TYR:CE2	1:C:252:MET:HB3	2.47	0.49
2:D:147:GLU:OE2	2:D:148:GLU:C	2.51	0.49
1:A:115:GLN:O	1:A:118:TYR:HB3	2.13	0.49
1:A:128:LEU:HD12	1:A:292:SER:N	2.27	0.49
2:B:143:ASN:OD1	2:B:145:PHE:HB2	2.13	0.49
2:D:54:ILE:O	2:D:58:VAL:HG23	2.13	0.49
1:C:51:LEU:HD13	1:C:52:ALA:N	2.27	0.49
1:A:159:ASN:O	1:A:159:ASN:ND2	2.39	0.49
1:A:164:THR:C	1:A:166:ASP:H	2.16	0.49
1:C:97:GLN:HE21	1:C:102:VAL:HG21	1.78	0.49
1:A:229:SER:CB	1:A:233:ASP:HB2	2.43	0.49
1:A:65:GLU:OE2	1:A:65:GLU:HA	2.12	0.49
1:A:97:GLN:HE21	1:A:102:VAL:HG21	1.78	0.49
2:B:97:GLN:O	2:B:100:LEU:HB2	2.12	0.49
1:A:78:VAL:CG1	2:B:135:ILE:HD11	2.42	0.49
1:A:202:GLN:HE22	1:A:262:GLY:C	2.17	0.48
1:C:222:GLU:HG2	1:C:223:LEU:N	2.25	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:GLU:OE1	2:D:150:GLU:HA	2.13	0.48
1:A:135:GLU:HB2	1:A:138:GLU:CG	2.42	0.48
1:C:186:ILE:O	1:C:267:PHE:HA	2.13	0.48
1:C:52:ALA:HB1	1:C:81:ARG:HH12	1.78	0.48
1:A:61:ARG:HH11	1:A:61:ARG:CB	2.17	0.48
2:D:147:GLU:OE2	2:D:148:GLU:O	2.31	0.48
2:D:25:VAL:O	2:D:29:THR:HG23	2.12	0.48
1:A:66:LEU:HB2	1:A:71:LEU:HD21	1.95	0.48
2:B:100:LEU:O	2:B:103:LEU:N	2.43	0.48
2:B:116:LEU:HA	2:B:119:THR:HG22	1.96	0.48
1:C:140:TRP:CE3	1:C:182:LYS:HD2	2.48	0.48
2:D:85:ILE:HB	2:D:118:VAL:HG23	1.96	0.48
1:A:288:VAL:O	1:A:289:THR:HB	2.13	0.48
2:B:134:GLU:O	2:B:137:LYS:HB3	2.13	0.48
1:A:159:ASN:ND2	1:A:159:ASN:C	2.61	0.48
1:A:207:VAL:HG11	1:A:225:VAL:HG21	1.95	0.48
2:B:149:GLU:O	2:B:150:GLU:C	2.51	0.48
2:B:21:ALA:O	2:B:22:LYS:HB3	2.14	0.48
1:C:229:SER:CB	1:C:233:ASP:HB2	2.43	0.48
2:D:137:LYS:HD3	2:D:138:THR:CG2	2.43	0.48
2:B:150:GLU:OE2	2:B:152:GLN:HB3	2.13	0.48
2:D:146:THR:HB	2:D:147:GLU:H	1.51	0.48
2:D:17:ASP:OD1	2:D:19:GLU:HB3	2.14	0.48
2:B:21:ALA:O	2:B:23:GLN:N	2.47	0.47
1:C:278:VAL:O	1:C:279:TYR:CB	2.61	0.47
1:A:210:TRP:HD1	1:A:290:ASN:HD22	1.62	0.47
1:A:264:GLY:O	1:A:266:ARG:HG2	2.15	0.47
1:A:83:LYS:C	1:A:85:LEU:N	2.68	0.47
1:C:150:TRP:CE2	1:C:180:CYS:HB3	2.50	0.47
1:A:81:ARG:HA	1:A:84:GLU:OE2	2.14	0.47
1:C:177:PHE:CE2	1:C:281:LYS:HA	2.49	0.47
1:A:114:TRP:O	1:A:115:GLN:C	2.51	0.47
2:D:91:GLU:O	2:D:94:LYS:HB2	2.14	0.47
1:C:101:LEU:CD2	1:C:121:SER:HB3	2.43	0.47
1:C:94:LEU:O	1:C:96:CYS:N	2.48	0.47
1:C:128:LEU:HD12	1:C:291:SER:C	2.35	0.47
1:C:68:ALA:O	1:C:69:THR:C	2.53	0.47
1:C:96:CYS:O	1:C:99:GLU:N	2.47	0.47
1:C:157:GLY:HA3	1:C:287:ARG:HH12	1.80	0.47
1:C:76:ARG:HD2	1:C:87:ASP:OD1	2.15	0.47
1:A:157:GLY:N	1:A:160:GLY:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:GLU:O	2:B:33:ASP:CB	2.63	0.47
2:B:25:VAL:O	2:B:29:THR:HG23	2.14	0.46
1:A:194:TRP:CZ2	1:A:197:LEU:HD22	2.50	0.46
2:B:17:ASP:O	2:B:20:ILE:HD13	2.14	0.46
1:A:211:TYR:CE2	1:A:252:MET:HB3	2.50	0.46
1:C:177:PHE:HA	1:C:276:ASP:OD1	2.16	0.46
2:D:119:THR:CG2	2:D:120:CYS:N	2.78	0.46
1:A:259:ILE:O	1:A:260:ASP:C	2.54	0.46
1:A:177:PHE:CD2	1:A:281:LYS:HA	2.51	0.46
2:B:55:LEU:O	2:B:59:ILE:HG23	2.16	0.46
1:C:228:LEU:HB2	1:C:267:PHE:HB2	1.98	0.46
1:A:210:TRP:CD1	1:A:290:ASN:ND2	2.82	0.46
1:C:155:LEU:HD11	1:C:163:PHE:HB2	1.98	0.46
2:D:56:LYS:HG3	2:D:60:GLN:HE21	1.80	0.46
1:A:122:LYS:HD2	1:A:122:LYS:HA	1.73	0.46
1:A:66:LEU:HA	1:A:67:PRO:HD2	1.66	0.46
2:B:116:LEU:O	2:B:116:LEU:HD12	2.16	0.46
2:B:119:THR:CG2	2:B:120:CYS:N	2.78	0.46
1:A:63:LEU:C	1:A:65:GLU:H	2.20	0.46
1:C:83:LYS:C	1:C:85:LEU:N	2.68	0.46
1:A:76:ARG:HD2	1:A:87:ASP:OD1	2.15	0.45
1:A:76:ARG:NH1	1:A:87:ASP:OD2	2.49	0.45
2:B:137:LYS:HD3	2:B:138:THR:CG2	2.46	0.45
2:D:124:ALA:HA	2:D:127:ILE:HG13	1.98	0.45
2:D:24:SER:HA	2:D:112:ILE:HG12	1.98	0.45
1:A:51:LEU:CD1	1:A:52:ALA:N	2.80	0.45
2:B:12:GLU:HG2	2:B:13:ILE:N	2.31	0.45
2:B:16:VAL:HB	2:B:20:ILE:HD11	1.97	0.45
2:D:100:LEU:O	2:D:103:LEU:HB2	2.17	0.45
1:C:220:LEU:HA	1:C:245:VAL:HG23	1.99	0.45
1:C:66:LEU:HA	1:C:67:PRO:HD2	1.68	0.45
2:B:64:HIS:CE1	2:D:128:LYS:CE	2.62	0.45
2:D:132:PRO:O	2:D:133:GLU:C	2.54	0.45
2:D:9:SER:HA	2:D:48:PRO:HA	1.97	0.45
1:A:55:PRO:O	1:A:56:GLU:C	2.55	0.45
2:D:85:ILE:HG13	2:D:90:GLN:HG2	1.98	0.45
1:A:130:ASN:HB2	1:A:135:GLU:OE1	2.17	0.45
2:D:150:GLU:OE2	2:D:152:GLN:HB3	2.16	0.45
2:D:22:LYS:HG3	2:D:28:LYS:CG	2.47	0.45
1:A:62:VAL:O	1:A:65:GLU:HB2	2.17	0.45
2:B:4:ILE:N	2:B:16:VAL:O	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:GLU:HB3	1:C:57:PRO:CD	2.47	0.45
2:D:103:LEU:O	2:D:105:LEU:N	2.50	0.45
2:D:65:HIS:C	2:D:67:ASP:N	2.70	0.45
1:C:164:THR:C	1:C:166:ASP:H	2.17	0.44
1:C:180:CYS:O	1:C:273:GLY:HA3	2.18	0.44
2:D:126:MET:O	2:D:130:LYS:CE	2.65	0.44
2:B:126:MET:HE2	2:B:139:PHE:CZ	2.52	0.44
1:C:89:ALA:O	1:C:93:LEU:HB2	2.16	0.44
1:A:69:THR:HG22	1:A:73:GLN:NE2	2.33	0.44
2:B:9:SER:HA	2:B:48:PRO:HA	2.00	0.44
2:D:20:ILE:C	2:D:21:ALA:O	2.54	0.44
2:B:87:VAL:HG11	1:C:69:THR:CG2	2.48	0.44
2:D:21:ALA:O	2:D:22:LYS:CB	2.65	0.44
2:B:148:GLU:OE1	2:B:150:GLU:HA	2.16	0.44
2:B:97:GLN:O	2:B:100:LEU:N	2.50	0.44
1:A:179:TRP:CZ2	1:A:242:GLN:HG2	2.53	0.44
1:C:157:GLY:N	1:C:160:GLY:O	2.51	0.44
1:A:79:CYS:SG	1:A:80:LEU:N	2.88	0.44
1:C:115:GLN:O	1:C:118:TYR:HB3	2.18	0.44
2:D:54:ILE:HG13	2:D:102:GLU:HB3	1.99	0.44
1:A:259:ILE:O	1:A:261:TYR:N	2.51	0.44
2:D:61:TRP:HD1	2:D:92:PHE:CD2	2.36	0.44
1:A:155:LEU:HD11	1:A:163:PHE:HB2	1.98	0.43
2:B:131:THR:O	2:B:132:PRO:C	2.55	0.43
1:C:55:PRO:O	1:C:56:GLU:C	2.56	0.43
2:D:148:GLU:OE1	2:D:150:GLU:CA	2.65	0.43
1:C:52:ALA:CB	1:C:81:ARG:HH12	2.30	0.43
2:D:55:LEU:O	2:D:59:ILE:CG2	2.66	0.43
2:B:14:PHE:CD2	2:B:55:LEU:HD23	2.54	0.43
1:C:131:PRO:HB3	1:C:291:SER:O	2.17	0.43
2:B:18:VAL:O	2:B:22:LYS:HB2	2.18	0.43
1:C:275:GLN:HA	1:C:285:GLY:HA3	2.00	0.43
1:A:101:LEU:CD2	1:A:121:SER:HB3	2.44	0.43
2:D:26:THR:HG21	2:D:109:TYR:O	2.18	0.43
2:D:55:LEU:O	2:D:58:VAL:HB	2.18	0.43
1:A:101:LEU:H	1:A:101:LEU:HG	1.53	0.43
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.81	0.43
2:B:131:THR:H	2:B:134:GLU:HB2	1.84	0.43
2:B:20:ILE:C	2:B:21:ALA:O	2.52	0.43
2:B:59:ILE:HD13	2:B:60:GLN:N	2.33	0.43
1:C:130:ASN:HB2	1:C:135:GLU:OE1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:LEU:O	2:D:103:LEU:N	2.44	0.43
2:D:27:ILE:HD12	2:D:27:ILE:O	2.18	0.43
1:A:224:THR:HA	1:A:238:PHE:O	2.19	0.43
1:A:231:ASN:O	1:A:232:GLU:C	2.56	0.43
1:A:82:TRP:O	1:A:86:VAL:HG23	2.17	0.43
1:C:179:TRP:CZ2	1:C:242:GLN:HG2	2.54	0.43
2:D:109:TYR:CD1	2:D:109:TYR:C	2.92	0.43
2:B:88:TRP:O	2:B:91:GLU:HB3	2.18	0.43
1:C:114:TRP:O	1:C:115:GLN:C	2.56	0.43
2:B:130:LYS:NZ	2:B:138:THR:HG21	2.34	0.43
1:C:278:VAL:O	1:C:279:TYR:HB3	2.18	0.43
2:D:17:ASP:HB3	2:D:20:ILE:HD12	2.01	0.43
1:A:177:PHE:HA	1:A:276:ASP:OD1	2.18	0.43
1:A:56:GLU:N	1:A:57:PRO:HD2	2.34	0.43
2:D:48:PRO:HD2	2:D:49:ASN:HD22	1.84	0.43
1:A:170:LYS:HB2	1:A:171:LYS:HG3	2.01	0.42
1:C:197:LEU:HD12	1:C:201:THR:HB	2.01	0.42
1:C:210:TRP:NE1	1:C:290:ASN:ND2	2.67	0.42
1:C:227:LEU:HD12	1:C:236:ALA:CB	2.41	0.42
2:D:52:ALA:HA	2:D:55:LEU:HB3	2.02	0.42
2:B:148:GLU:OE1	2:B:150:GLU:CA	2.68	0.42
2:B:56:LYS:O	2:B:60:GLN:HG3	2.18	0.42
1:C:212:SER:OG	1:C:287:ARG:HD2	2.18	0.42
1:C:65:GLU:OE2	1:C:65:GLU:CA	2.63	0.42
2:D:98:GLY:O	2:D:99:THR:C	2.58	0.42
1:A:178:GLU:O	1:A:275:GLN:HB3	2.19	0.42
2:B:87:VAL:HG11	1:C:69:THR:HG22	2.01	0.42
1:C:119:PHE:O	1:C:122:LYS:HB2	2.20	0.42
1:C:128:LEU:HD12	1:C:292:SER:N	2.34	0.42
1:C:163:PHE:CD2	1:C:169:VAL:CG2	2.97	0.42
1:A:94:LEU:O	1:A:95:LYS:C	2.56	0.42
2:B:65:HIS:C	2:B:67:ASP:H	2.23	0.42
1:C:122:LYS:HA	1:C:122:LYS:HD2	1.71	0.42
1:C:296:GLU:HA	1:C:297:PRO:HD2	1.90	0.42
1:C:59:LEU:HA	1:C:59:LEU:HD12	1.86	0.42
1:C:82:TRP:HH2	2:D:127:ILE:HD13	1.85	0.42
1:A:227:LEU:HD11	1:A:258:PHE:CD1	2.55	0.42
1:A:259:ILE:HD13	1:A:259:ILE:O	2.20	0.42
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.85	0.42
2:D:136:ARG:HA	2:D:141:ILE:CG2	2.49	0.42
1:A:83:LYS:C	1:A:85:LEU:H	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ASN:ND2	1:C:159:ASN:C	2.74	0.41
1:A:290:ASN:O	1:A:290:ASN:ND2	2.53	0.41
1:A:155:LEU:HA	1:A:155:LEU:HD23	1.80	0.41
1:A:56:GLU:O	1:A:60:LEU:HD22	2.20	0.41
1:C:287:ARG:HE	1:C:287:ARG:HB3	1.58	0.41
1:A:135:GLU:O	1:A:136:ASP:C	2.57	0.41
1:C:270:PHE:CD2	1:C:270:PHE:C	2.94	0.41
1:A:96:CYS:O	1:A:99:GLU:N	2.47	0.41
2:B:117:ASP:OD2	2:B:121:LYS:CE	2.59	0.41
2:B:27:ILE:O	2:B:30:MET:HB3	2.21	0.41
1:A:199:ASP:HB3	1:A:263:PRO:HB3	2.03	0.41
2:D:115:LEU:O	2:D:118:VAL:HG12	2.21	0.41
2:D:12:GLU:HG2	2:D:13:ILE:N	2.36	0.41
1:A:94:LEU:O	1:A:96:CYS:N	2.54	0.41
1:C:162:GLU:HG3	1:C:163:PHE:H	1.86	0.41
1:A:64:ALA:HB2	1:A:94:LEU:HD23	2.03	0.41
1:A:71:LEU:HD13	1:A:91:LEU:HD11	2.01	0.41
2:B:29:THR:O	2:B:32:GLU:O	2.39	0.41
1:C:143:VAL:HA	1:C:181:ARG:O	2.21	0.41
2:D:116:LEU:O	2:D:116:LEU:HD12	2.21	0.41
1:A:100:GLY:O	1:A:102:VAL:N	2.54	0.41
1:A:135:GLU:O	1:A:138:GLU:HB2	2.21	0.41
2:B:104:ILE:HB	2:B:119:THR:HG23	2.03	0.41
2:B:112:ILE:C	2:B:114:GLY:N	2.74	0.41
1:C:63:LEU:O	1:C:65:GLU:N	2.54	0.41
2:D:18:VAL:HG12	2:D:22:LYS:HD2	2.03	0.41
1:A:59:LEU:HA	1:A:59:LEU:HD12	1.61	0.40
1:A:78:VAL:HG21	2:B:135:ILE:HD11	2.03	0.40
1:C:129:ARG:CG	1:C:129:ARG:HH11	2.34	0.40
1:C:259:ILE:HD13	1:C:259:ILE:O	2.21	0.40
2:D:54:ILE:O	2:D:55:LEU:C	2.60	0.40
1:A:223:LEU:HD13	1:A:272:HIS:HB3	2.03	0.40
1:A:63:LEU:C	1:A:65:GLU:N	2.73	0.40
1:C:50:TYR:HA	1:C:53:GLU:OE1	2.21	0.40
2:D:119:THR:HG23	2:D:120:CYS:N	2.35	0.40
2:B:147:GLU:HB2	2:B:148:GLU:H	1.49	0.40
2:B:87:VAL:HA	2:B:90:GLN:HG3	2.02	0.40
1:C:60:LEU:N	1:C:60:LEU:HD22	2.35	0.40
2:D:14:PHE:CE2	2:D:55:LEU:HD23	2.56	0.40
1:A:211:TYR:HA	1:A:287:ARG:O	2.21	0.40
1:A:63:LEU:O	1:A:64:ALA:C	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ASN:ND2	2:B:51:ASN:C	2.75	0.40
2:B:49:ASN:N	2:B:49:ASN:ND2	2.70	0.40
2:D:147:GLU:HB2	2:D:148:GLU:H	1.49	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:A:165:GLN:NE2	2:B:33:ASP:O[4_455]	2.09	0.11

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	236/297 (80%)	188 (80%)	32 (14%)	16 (7%)	1	16
1	C	236/297 (80%)	185 (78%)	36 (15%)	15 (6%)	1	18
2	B	124/166 (75%)	90 (73%)	21 (17%)	13 (10%)	0	7
2	D	124/166 (75%)	90 (73%)	20 (16%)	14 (11%)	0	6
All	All	720/926 (78%)	553 (77%)	109 (15%)	58 (8%)	1	12

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	136	ASP
1	A	143	VAL
1	A	230	GLU
1	A	260	ASP
2	B	11	GLY
2	B	84	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	144	ASP
2	B	146	THR
1	C	136	ASP
1	C	143	VAL
1	C	230	GLU
1	C	247	GLU
1	C	260	ASP
2	D	11	GLY
2	D	144	ASP
2	D	146	THR
2	D	147	GLU
1	A	51	LEU
1	A	52	ALA
1	A	64	ALA
1	A	124	ARG
1	A	247	GLU
1	A	279	TYR
2	B	97	GLN
2	B	98	GLY
2	B	147	GLU
1	C	101	LEU
1	C	124	ARG
1	C	158	ASP
1	C	279	TYR
2	D	97	GLN
1	A	95	LYS
2	B	100	LEU
2	B	150	GLU
1	C	52	ALA
1	C	291	SER
2	D	21	ALA
2	D	66	LYS
2	D	90	GLN
2	D	98	GLY
2	D	150	GLU
1	A	84	GLU
1	A	166	ASP
2	B	21	ALA
2	B	85	ILE
1	C	96	CYS
2	D	85	ILE
2	D	148	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	CYS
2	B	148	GLU
2	D	3	SER
1	A	142	ASP
2	B	104	ILE
1	C	165	GLN
2	D	58	VAL
1	C	246	PRO
1	C	56	GLU

5.3.2 Protein sidechains ⓘ

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	206/250 (82%)	167 (81%)	39 (19%)	2	9
1	C	206/250 (82%)	168 (82%)	38 (18%)	2	10
2	B	119/152 (78%)	91 (76%)	28 (24%)	1	5
2	D	119/152 (78%)	85 (71%)	34 (29%)	0	3
All	All	650/804 (81%)	511 (79%)	139 (21%)	1	6

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	61	ARG
1	A	65	GLU
1	A	69	THR
1	A	73	GLN
1	A	77	LEU
1	A	79	CYS
1	A	81	ARG
1	A	84	GLU
1	A	93	LEU
1	A	99	GLU
1	A	113	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	121	SER
1	A	124	ARG
1	A	129	ARG
1	A	130	ASN
1	A	138	GLU
1	A	144	GLU
1	A	158	ASP
1	A	159	ASN
1	A	161	VAL
1	A	167	ASP
1	A	169	VAL
1	A	184	GLN
1	A	200	THR
1	A	202	GLN
1	A	214	ARG
1	A	215	THR
1	A	222	GLU
1	A	224	THR
1	A	229	SER
1	A	247	GLU
1	A	250	SER
1	A	252	MET
1	A	255	SER
1	A	259	ILE
1	A	260	ASP
1	A	272	HIS
1	A	291	SER
2	B	8	SER
2	B	13	ILE
2	B	20	ILE
2	B	24	SER
2	B	27	ILE
2	B	31	LEU
2	B	43	ASP
2	B	49	ASN
2	B	50	VAL
2	B	51	ASN
2	B	59	ILE
2	B	63	THR
2	B	66	LYS
2	B	68	ASP
2	B	104	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	105	LEU
2	B	113	LYS
2	B	121	LYS
2	B	127	ILE
2	B	135	ILE
2	B	141	ILE
2	B	142	LYS
2	B	144	ASP
2	B	146	THR
2	B	147	GLU
2	B	150	GLU
2	B	152	GLN
2	B	154	ARG
1	C	53	GLU
1	C	61	ARG
1	C	65	GLU
1	C	69	THR
1	C	72	VAL
1	C	77	LEU
1	C	79	CYS
1	C	81	ARG
1	C	84	GLU
1	C	99	GLU
1	C	113	HIS
1	C	124	ARG
1	C	129	ARG
1	C	130	ASN
1	C	138	GLU
1	C	144	GLU
1	C	158	ASP
1	C	159	ASN
1	C	161	VAL
1	C	163	PHE
1	C	167	ASP
1	C	168	SER
1	C	169	VAL
1	C	197	LEU
1	C	200	THR
1	C	202	GLN
1	C	214	ARG
1	C	215	THR
1	C	222	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	224	THR
1	C	229	SER
1	C	250	SER
1	C	252	MET
1	C	255	SER
1	C	259	ILE
1	C	260	ASP
1	C	272	HIS
1	C	291	SER
2	D	5	LYS
2	D	8	SER
2	D	13	ILE
2	D	20	ILE
2	D	24	SER
2	D	27	ILE
2	D	30	MET
2	D	31	LEU
2	D	43	ASP
2	D	49	ASN
2	D	50	VAL
2	D	51	ASN
2	D	59	ILE
2	D	63	THR
2	D	66	LYS
2	D	67	ASP
2	D	68	ASP
2	D	85	ILE
2	D	104	ILE
2	D	105	LEU
2	D	108	ASN
2	D	120	CYS
2	D	121	LYS
2	D	127	ILE
2	D	135	ILE
2	D	137	LYS
2	D	141	ILE
2	D	142	LYS
2	D	144	ASP
2	D	147	GLU
2	D	148	GLU
2	D	150	GLU
2	D	152	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	154	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	97	GLN
1	A	98	GLN
1	A	113	HIS
1	A	116	GLN
1	A	130	ASN
1	A	159	ASN
1	A	202	GLN
1	A	242	GLN
1	A	290	ASN
2	B	49	ASN
2	B	51	ASN
2	B	60	GLN
2	B	64	HIS
2	B	108	ASN
1	C	97	GLN
1	C	98	GLN
1	C	113	HIS
1	C	130	ASN
1	C	159	ASN
1	C	202	GLN
1	C	242	GLN
2	D	49	ASN
2	D	51	ASN
2	D	60	GLN
2	D	97	GLN
2	D	108	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [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	240/297 (80%)	-0.05	3 (1%) 77 69	31, 50, 66, 71	0
1	C	240/297 (80%)	-0.15	0 100 100	31, 49, 67, 71	0
2	B	130/166 (78%)	-0.00	3 (2%) 61 51	31, 52, 70, 82	0
2	D	130/166 (78%)	-0.20	0 100 100	31, 52, 70, 82	0
All	All	740/926 (79%)	-0.10	6 (0%) 86 79	31, 51, 67, 82	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	7	GLN	3.4
2	B	2	PRO	2.4
1	A	171	LYS	2.3
2	B	6	LEU	2.1
1	A	162	GLU	2.1
1	A	163	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.