



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:31 PM UTC

PDB ID : 4J1U / pdb_00004j1u
Title : Crystal structure of antibody 93F3 unstable variant
Authors : Wang, F.
Deposited on : 2013-02-02
Resolution : 2.58 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:

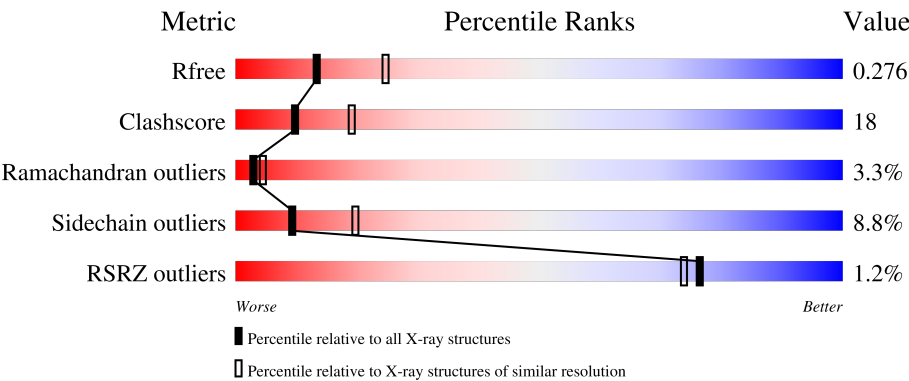
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	219	66%26%... .
1	C	219	61%33%... .
1	E	219	% 60%32%5%..
2	B	238	63%19%5%13%
2	D	238	3% 45%37%6%.12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	238	2% 62% 22% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9570 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 antibody 93F3 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1610	1011	264	329	6			
1	C	213	Total	C	N	O	S	0	0	0
			1630	1017	273	334	6			
1	E	214	Total	C	N	O	S	0	0	0
			1644	1028	278	332	6			

- Molecule 2 is a protein called antibody 93F3 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1530	968	251	305	6			
2	D	210	Total	C	N	O	S	0	0	0
			1547	981	254	306	6			
2	F	207	Total	C	N	O	S	0	0	0
			1531	970	252	303	6			

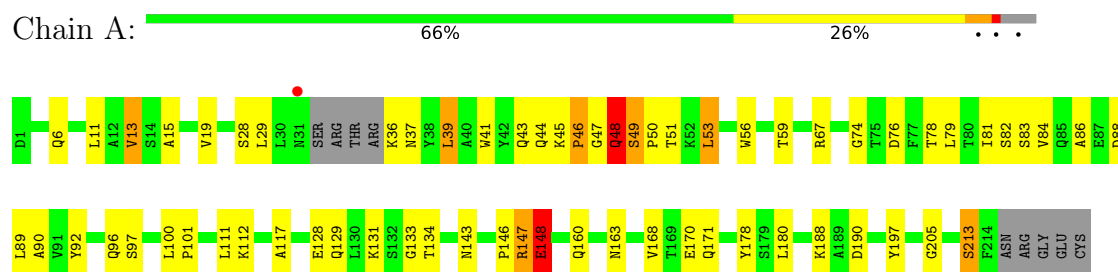
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	8	Total	O	0	0
			8	8		
3	C	25	Total	O	0	0
			25	25		
3	D	8	Total	O	0	0
			8	8		
3	E	11	Total	O	0	0
			11	11		
3	F	16	Total	O	0	0
			16	16		

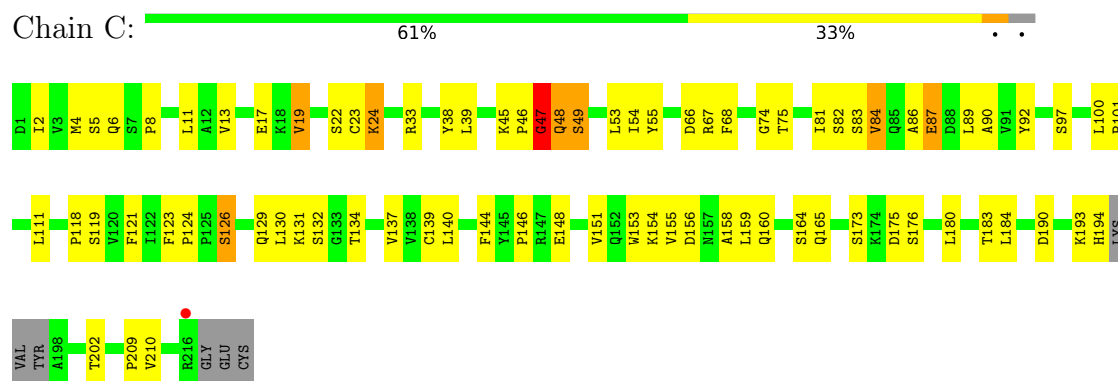
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

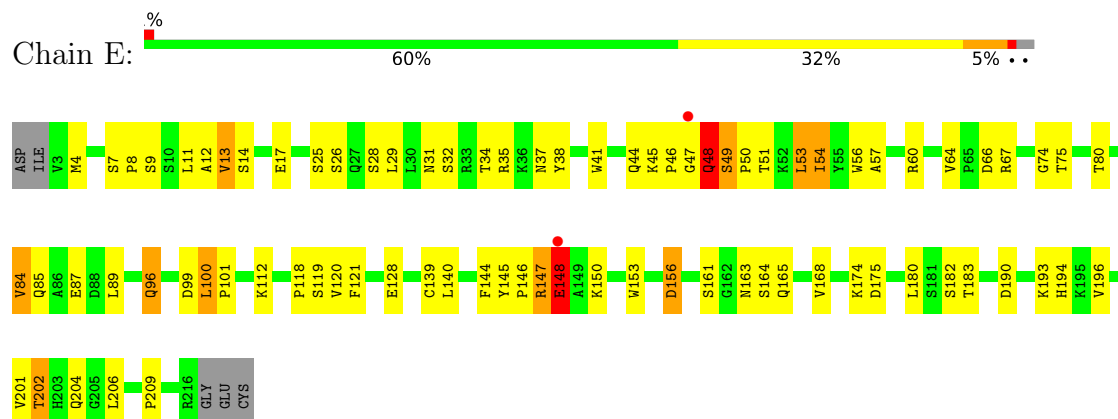
- Molecule 1: antibody 93F3 Light chain



- Molecule 1: antibody 93F3 Light chain



- Molecule 1: antibody 93F3 Light chain



Chain B:

Residue Type	Count
VAL	1
ASP	1
TYR	1
LYS	1
ASP	1
ASP	1
ASP	1
ASP	1
LYS	1
HIS	1
HIS	1
HIS	1
HIS	1
HIS	1
SER	1
THR	1
SER	1
G137	1
G138	1
T139	1
L142	1
L145	1
D148	1
P151	1
E152	1
P153	1
V154	1
T155	1
V156	1
S157	1
S160	1
G161	1
A162	1
L163	1
F170	1
S181	1
L182	1
S183	1
S190	1
S191	1
S192	1
Q196	1
I199	1
C200	1
N201	1
V202	1
N203	1
H204	1
K205	1
P206	1
T209	1
D212	1
K213	1
K214	1
P217	1
LYS	1
SER	1
CYS	1
ASP	1
LYS	1
ASP	1

Chain D:

3% 45% 37% 6% 12%

Label	Color
GLN	Grey
V2	Green
P9	Green
G10	Green
L11	Green
V12	Green
A13	Green
P14	Orange
S15	Yellow
Q16	Yellow
S17	Yellow
I20	Yellow
T21	Green
C22	Yellow
T23	Yellow
V24	Yellow
G26	Green
F27	Orange
S28	Yellow
L29	Yellow
G33	Yellow
Q39	Yellow
P40	Yellow
P41	Green
G42	Green
K43	Green
G44	Green
L45	Green
E46	Green
W47	Green
W52	Yellow
G53	Yellow
S56	Yellow
Y59	Yellow
L63	Yellow
K64	Yellow
S65	Yellow
R66	Yellow
L67	Yellow
S68	Green
I69	Yellow
S70	Yellow
K71	Yellow
D72	Green
N73	Yellow
Q77	Yellow
V78	Yellow
F79	Yellow
L80	Yellow
V81	Yellow
M82	Yellow
N83	Yellow
S84	Green
L85	Yellow
Q86	Yellow
T87	Yellow
D88	Green
T89	Yellow
T90	Yellow
A91	Yellow
M92	Green
Y93	Yellow
K97	Yellow
H98	Green
T99	Yellow
Y100	Yellow
G101	Green
G102	Green
P103	Green
G104	Yellow
D105	Yellow
T111	Yellow
S112	Yellow
V113	Red
T114	Yellow
V115	Yellow
T120	Yellow
V125	Yellow
F126	Yellow
P127	Yellow
P130	Yellow
SER	Grey
SER	Grey
LYS	Grey
SER	Grey
THR	Grey
SER	Grey
G137	Green
A141	Yellow
L142	Orange
S65	Yellow
G143	Yellow
C144	Yellow
L145	Green
V146	Yellow
K147	Yellow
D148	Red
P151	Yellow
E152	Green
P153	Yellow
V154	Orange
T155	Yellow
LYS	Yellow
V156	Yellow
F157	Yellow
W158	Yellow
M159	Yellow
S160	Yellow
G161	Orange
A162	Green
L163	Yellow
T164	Yellow
A172	Yellow
V173	Yellow
L174	Yellow
Q175	Yellow
L179	Yellow
V180	Yellow
S181	Yellow
L182	Yellow
V185	Yellow
V186	Yellow
S190	Yellow
S191	Yellow
S192	Yellow
T195	Yellow
Q196	Yellow
T197	Green
Y198	Yellow
I199	Yellow
C200	Yellow
N201	Yellow
V202	Yellow
N203	Yellow
N204	Green
K205	Yellow
F206	Yellow
V211	Yellow
D212	Yellow
K213	Yellow
F217	Green
LYS	Grey
SER	Grey
CYS	Yellow
ASP	Grey
LYS	Grey
ASP	Grey
VAL	Grey
ASP	Grey
TYR	Grey
LYS	Grey
ASP	Grey
ASP	Grey
ASP	Grey
ASP	Grey
LYS	Grey
HIS	Grey
HIS	Grey

Chain F:

Amino Acid	Count
ASP	1
VAL	1
G108	1
ASP	1
TYR	1
LYS	1
ASP	1
ASP	1
ASP	1
LYS	1
HIS	1
HIS	1
HIS	1
HIS	1
HIS	1
HIS	1
W107	1
G108	1
G109	1
G110	1
V115	1
T120	1
K121	1
L128	1
A129	1
P130	1
SER	1
SER	1
LYS	1
LYS	1
THR	1
S136	1
T139	1
A140	1
A141	1
L142	1
G143	1
D148	1
Y149	1
P153	1
V154	1
L163	1
H168	1
A172	1
L182	1
S183	1
V188	1
P189	1
S190	1
L193	1
N201	1
S207	1
N208	1
T209	1
E216	1
P217	1
SER	1
CYS	1
ASP	1
LYS	1
GLN	1
V2	1
K5	1
E6	1
P14	1
S15	1
S16	1
S17	1
T20	1
T21	1
C22	1
T23	1
Y24	1
L29	1
T30	1
R38	1
W47	1
L48	1
G49	1
W52	1
S56	1
Y59	1
L67	1
S68	1
D72	1
N73	1
S74	1
K75	1
S76	1
L80	1
S84	1
T87	1
D88	1
D89	1
T90	1
K97	1
H98	1
T99	1
TYR	1
GLY	1
PRO	1
GLY	1
D105	1
E106	1

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.03Å 112.57Å 86.51Å 90.00° 115.28° 90.00°	Depositor
Resolution (Å)	78.33 – 2.58 78.22 – 2.58	Depositor EDS
% Data completeness (in resolution range)	94.8 (78.33-2.58) 94.8 (78.22-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.276 0.210 , 0.276	Depositor DCC
R_{free} test set	2121 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9570	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.81	0/1643	1.07	5/2228 (0.2%)
1	C	0.85	0/1662	1.08	4/2253 (0.2%)
1	E	1.01	3/1678 (0.2%)	1.28	15/2275 (0.7%)
2	B	0.85	0/1566	1.05	4/2133 (0.2%)
2	D	0.90	0/1586	1.13	9/2163 (0.4%)
2	F	0.94	2/1567 (0.1%)	1.08	6/2134 (0.3%)
All	All	0.90	5/9702 (0.1%)	1.12	43/13186 (0.3%)

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	2
1	E	0	2
2	D	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	35	ARG	NE-CZ	11.92	1.46	1.33
1	E	35	ARG	CZ-NH1	-9.57	1.19	1.32
2	F	168	HIS	CE1-NE2	5.43	1.38	1.32
2	F	168	HIS	CG-CD2	5.23	1.41	1.35
1	E	41	TRP	CA-C	-5.01	1.46	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	147	ARG	CA-C-N	12.80	144.74	121.70
1	E	147	ARG	C-N-CA	12.80	144.74	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	ARG	NE-CZ-NH2	11.71	129.74	119.20
1	E	147	ARG	N-CA-C	10.97	124.28	111.11
1	A	147	ARG	N-CA-C	8.86	120.55	111.07
1	E	148	GLU	N-CA-CB	8.16	124.36	110.50
2	D	154	VAL	N-CA-C	-8.11	97.16	108.27
1	E	35	ARG	NH1-CZ-NH2	-7.65	109.36	119.30
1	C	87	GLU	N-CA-C	-7.13	103.80	114.64
2	B	154	VAL	N-CA-C	-7.12	98.96	108.35
1	E	100	LEU	CA-C-N	6.95	126.92	119.76
1	E	100	LEU	C-N-CA	6.95	126.92	119.76
2	F	188	VAL	CA-C-N	-6.70	112.56	120.13
2	F	188	VAL	C-N-CA	-6.70	112.56	120.13
2	D	113	VAL	CA-C-N	6.58	133.54	121.70
2	D	113	VAL	C-N-CA	6.58	133.54	121.70
1	A	147	ARG	CA-C-N	6.46	133.33	121.70
1	A	147	ARG	C-N-CA	6.46	133.33	121.70
2	B	154	VAL	CA-C-N	6.42	133.26	121.70
2	B	154	VAL	C-N-CA	6.42	133.26	121.70
1	E	64	VAL	CA-C-N	6.17	127.55	119.84
1	E	64	VAL	C-N-CA	6.17	127.55	119.84
2	D	154	VAL	CA-C-N	6.15	132.77	121.70
2	D	154	VAL	C-N-CA	6.15	132.77	121.70
2	F	140	ALA	CA-C-N	5.92	132.35	121.70
2	F	140	ALA	C-N-CA	5.92	132.35	121.70
2	D	40	PRO	O-C-N	5.87	124.01	121.31
1	C	124	PRO	O-C-N	5.86	123.90	121.15
1	E	147	ARG	O-C-N	-5.85	116.01	122.09
1	C	47	GLY	CA-C-N	5.74	132.03	121.70
1	C	47	GLY	C-N-CA	5.74	132.03	121.70
2	D	161	GLY	N-CA-C	-5.67	107.95	114.69
2	B	40	PRO	O-C-N	5.65	123.81	121.15
1	E	147	ARG	CA-C-O	-5.62	114.88	120.90
1	A	48	GLN	CA-C-N	5.56	131.71	121.70
1	A	48	GLN	C-N-CA	5.56	131.71	121.70
1	E	48	GLN	CA-C-N	5.37	131.37	121.70
1	E	48	GLN	C-N-CA	5.37	131.37	121.70
2	F	193	LEU	N-CA-C	5.32	118.55	111.75
2	D	201	ASN	CA-C-N	5.13	130.94	121.70
2	D	201	ASN	C-N-CA	5.13	130.94	121.70
1	E	120	VAL	N-CA-C	5.05	115.37	107.99
2	F	30	THR	N-CA-C	-5.03	105.99	111.82

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	PRO	Peptide
1	A	48	GLN	Peptide
2	D	111	THR	Peptide
1	E	46	PRO	Peptide
1	E	48	GLN	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	1610	0	1573	48	0
1	C	1630	0	1588	73	0
1	E	1644	0	1609	64	0
2	B	1530	0	1509	35	0
2	D	1547	0	1519	90	0
2	F	1531	0	1511	35	0
3	A	10	0	0	0	0
3	B	8	0	0	0	0
3	C	25	0	0	1	0
3	D	8	0	0	0	0
3	E	11	0	0	0	0
3	F	16	0	0	1	0
All	All	9570	0	9309	331	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 18.

All (331) 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:A:147:ARG:N	1:A:148:GLU:HB2	1.50	1.23
1:E:147:ARG:N	1:E:148:GLU:HG2	1.59	1.15
1:E:4:MET:HE3	1:E:96:GLN:HB3	1.32	1.11
2:B:154:VAL:HA	2:B:155:THR:HG22	1.20	1.11
2:B:104:GLY:HA3	2:B:105:ASP:HB2	1.09	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:GLY:HA3	2:D:105:ASP:CB	1.86	1.05
2:F:87:THR:O	2:F:90:THR:HG23	1.56	1.05
1:A:47:GLY:HA2	1:A:48:GLN:O	1.56	1.05
1:E:193:LYS:HD3	1:E:194:HIS:CE1	1.94	1.03
2:D:104:GLY:CA	2:D:105:ASP:HB2	1.89	1.03
2:D:22:CYS:HB3	2:D:78:VAL:HG12	1.42	1.00
1:C:126:SER:N	2:D:126:PHE:HZ	1.58	1.00
2:D:104:GLY:HA3	2:D:105:ASP:HB2	1.00	0.99
2:B:104:GLY:CA	2:B:105:ASP:HB2	1.94	0.96
1:E:31:ASN:HB3	1:E:34:THR:HG22	1.45	0.96
2:D:163:LEU:HD21	2:D:186:VAL:HG21	1.44	0.96
1:C:81:ILE:HD13	1:C:84:VAL:HB	1.48	0.93
1:C:126:SER:N	2:D:126:PHE:CZ	2.38	0.90
2:D:154:VAL:HA	2:D:155:THR:HG22	1.53	0.89
1:C:47:GLY:HA2	1:C:48:GLN:O	1.74	0.87
1:E:4:MET:HE3	1:E:96:GLN:CB	2.05	0.86
2:B:104:GLY:HA3	2:B:105:ASP:CB	2.00	0.86
1:A:168:VAL:HG22	1:A:180:LEU:HD12	1.56	0.86
1:A:168:VAL:HG22	1:A:180:LEU:CD1	2.06	0.85
2:B:154:VAL:HA	2:B:155:THR:CG2	2.04	0.84
2:F:97:LYS:O	2:F:98:HIS:HB2	1.77	0.84
1:C:48:GLN:HA	1:C:49:SER:CB	2.08	0.84
2:D:201:ASN:HB3	2:D:212:ASP:OD1	1.77	0.84
1:C:202:THR:HG22	1:C:209:PRO:HG3	1.60	0.82
1:E:48:GLN:HA	1:E:49:SER:HB2	1.59	0.82
1:A:160:GLN:HB3	1:A:163:ASN:HD21	1.42	0.82
2:D:86:GLN:O	2:D:115:VAL:HG11	1.80	0.82
2:D:154:VAL:HA	2:D:155:THR:CG2	2.10	0.81
1:C:81:ILE:HD12	1:C:81:ILE:O	1.80	0.80
2:D:113:VAL:HA	2:D:114:THR:OG1	1.82	0.79
2:F:38:ARG:CD	2:F:48:LEU:HD21	2.13	0.78
2:D:199:ILE:HA	2:D:200:CYS:CB	2.15	0.77
1:A:128:GLU:O	1:A:131:LYS:HG2	1.84	0.77
2:B:199:ILE:HD11	2:B:212:ASP:HB3	1.67	0.77
2:D:90:THR:HG23	2:D:114:THR:H	1.49	0.76
1:E:47:GLY:HA3	1:E:48:GLN:O	1.86	0.76
1:C:126:SER:HB3	2:D:126:PHE:CE1	2.20	0.75
1:E:48:GLN:HA	1:E:49:SER:CB	2.13	0.75
1:E:121:PHE:HD2	1:E:140:LEU:HD12	1.51	0.75
1:E:147:ARG:CA	1:E:148:GLU:HG2	2.17	0.75
1:E:164:SER:HA	1:E:183:THR:O	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:VAL:CA	2:B:155:THR:HG22	2.10	0.75
1:C:119:SER:HB3	1:C:121:PHE:HE1	1.52	0.75
1:C:19:VAL:HG23	1:C:81:ILE:CG1	2.17	0.74
1:E:147:ARG:N	1:E:148:GLU:CG	2.47	0.74
1:A:147:ARG:CA	1:A:148:GLU:HB2	2.17	0.74
1:C:19:VAL:HG23	1:C:81:ILE:HG13	1.68	0.74
1:A:146:PRO:C	1:A:148:GLU:HB2	2.12	0.73
1:C:19:VAL:HG22	1:C:81:ILE:HD11	1.70	0.73
2:D:125:VAL:HG21	2:D:202:VAL:HG11	1.72	0.72
2:B:201:ASN:HB3	2:B:212:ASP:OD2	1.89	0.72
1:E:4:MET:CE	1:E:96:GLN:HG2	2.20	0.72
1:E:4:MET:CE	1:E:96:GLN:HB3	2.17	0.72
1:E:8:PRO:HG2	1:E:11:LEU:HG	1.72	0.71
2:D:87:THR:HA	2:D:115:VAL:CG1	2.21	0.71
1:C:81:ILE:CD1	1:C:84:VAL:HB	2.20	0.71
2:D:20:ILE:HD12	2:D:80:LEU:HD23	1.71	0.71
2:B:128:LEU:HD11	2:B:145:LEU:HB2	1.74	0.70
2:B:192:SER:HB2	2:B:196:GLN:HG3	1.73	0.69
1:A:67:ARG:HG3	1:A:82:SER:OG	1.92	0.69
2:B:155:THR:HG23	2:B:203:ASN:O	1.92	0.69
1:A:37:ASN:O	1:A:56:TRP:HA	1.94	0.68
2:D:155:THR:HG23	2:D:203:ASN:O	1.94	0.68
2:D:201:ASN:HA	2:D:202:VAL:HB	1.74	0.68
1:A:160:GLN:HE21	1:A:163:ASN:ND2	1.91	0.68
1:C:19:VAL:CG2	1:C:81:ILE:HD11	2.24	0.68
1:E:67:ARG:NH2	1:E:85:GLN:HG2	2.09	0.68
2:B:160:SER:HA	2:B:201:ASN:HD21	1.60	0.67
2:D:199:ILE:HA	2:D:200:CYS:HB3	1.76	0.67
1:C:81:ILE:HD13	1:C:84:VAL:CB	2.25	0.67
2:D:130:PRO:HG3	2:D:142:LEU:HB3	1.77	0.66
1:E:4:MET:HE2	1:E:96:GLN:HG2	1.76	0.66
1:C:48:GLN:HA	1:C:49:SER:HB3	1.78	0.66
2:D:114:THR:HG21	2:D:151:PRO:HB2	1.78	0.66
1:A:133:GLY:HA2	1:A:188:LYS:HB2	1.77	0.66
1:C:55:TYR:CD2	2:D:102:GLY:HA2	2.31	0.66
2:D:154:VAL:CA	2:D:155:THR:HG22	2.26	0.65
1:A:47:GLY:HA2	1:A:48:GLN:C	2.20	0.65
1:C:67:ARG:HD2	1:C:83:SER:O	1.96	0.65
2:F:38:ARG:HD2	2:F:48:LEU:HD21	1.77	0.65
1:A:43:GLN:HG3	1:A:92:TYR:CE2	2.31	0.65
1:E:4:MET:HE3	1:E:96:GLN:CG	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:ALA:HA	2:F:141:ALA:CB	2.28	0.64
2:B:154:VAL:HG13	2:B:203:ASN:O	1.97	0.64
1:C:87:GLU:HG3	1:C:173:SER:O	1.97	0.64
1:C:68:PHE:CD1	1:C:81:ILE:HG22	2.33	0.63
1:A:46:PRO:HG3	1:A:170:GLU:HG2	1.79	0.63
1:C:155:VAL:HG22	1:C:160:GLN:NE2	2.14	0.63
2:D:154:VAL:HG12	2:D:155:THR:O	1.98	0.63
2:B:157:SER:OG	2:B:201:ASN:ND2	2.32	0.63
1:A:28:SER:HA	1:A:74:GLY:O	1.98	0.63
1:A:89:LEU:HD21	1:A:171:GLN:HB3	1.80	0.63
1:C:137:VAL:HG13	1:C:184:LEU:HB3	1.81	0.63
2:D:174:LEU:HD13	2:D:180:TYR:CE2	2.34	0.62
1:A:13:VAL:CG1	1:A:84:VAL:HG11	2.29	0.62
1:C:48:GLN:HA	1:C:49:SER:HB2	1.81	0.62
1:A:147:ARG:H	1:A:148:GLU:HB2	1.56	0.61
2:D:12:VAL:HG21	2:D:85:LEU:HD13	1.82	0.61
2:F:38:ARG:HD3	2:F:48:LEU:HD21	1.82	0.61
2:D:172:ALA:HA	2:D:182:LEU:HB3	1.81	0.61
1:C:33:ARG:NH2	3:C:307:HOH:O	2.34	0.60
2:D:199:ILE:HA	2:D:200:CYS:HB2	1.83	0.60
2:F:90:THR:HG22	2:F:115:VAL:H	1.66	0.60
1:A:89:LEU:HB2	1:A:111:LEU:HD23	1.83	0.60
1:C:154:LYS:HA	1:C:158:ALA:O	2.01	0.60
1:A:160:GLN:HB3	1:A:163:ASN:ND2	2.15	0.60
1:E:139:CYS:HB3	1:E:182:SER:HB3	1.85	0.59
2:F:38:ARG:NH2	2:F:89:ASP:HA	2.18	0.59
1:E:31:ASN:HB3	1:E:34:THR:CG2	2.26	0.59
2:F:38:ARG:HH22	2:F:89:ASP:HA	1.67	0.59
1:C:38:TYR:HB3	1:C:97:SER:HB3	1.84	0.59
2:D:148:ASP:HA	2:D:180:TYR:O	2.03	0.59
2:B:160:SER:HA	2:B:201:ASN:ND2	2.18	0.59
1:E:17:GLU:O	1:E:84:VAL:HG12	2.03	0.58
1:C:175:ASP:OD1	1:C:175:ASP:O	2.21	0.58
1:E:168:VAL:CG1	1:E:180:LEU:HD12	2.33	0.58
2:B:19:SER:OG	2:B:81:LYS:HD3	2.02	0.58
2:B:21:THR:HG22	2:B:79:PHE:HD2	1.68	0.58
2:D:147:LYS:HA	2:D:181:SER:HB2	1.86	0.58
1:A:43:GLN:HB2	1:A:53:LEU:HD22	1.86	0.57
1:C:6:GLN:NE2	1:C:92:TYR:O	2.38	0.57
1:C:126:SER:CB	2:D:126:PHE:CE1	2.88	0.57
2:D:12:VAL:HG23	2:D:115:VAL:HG23	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ARG:H	1:E:148:GLU:HG2	1.59	0.57
1:C:165:GLN:HE22	2:D:175:GLN:NE2	2.03	0.57
2:F:20:ILE:HD12	2:F:80:LEU:HD23	1.86	0.56
1:C:180:LEU:HD23	1:C:180:LEU:C	2.30	0.56
2:D:13:ALA:O	2:D:16:GLN:HB2	2.05	0.56
1:A:147:ARG:HA	1:A:178:TYR:CD1	2.40	0.56
1:C:154:LYS:HZ2	1:C:159:LEU:HB2	1.70	0.56
1:E:153:TRP:CD1	1:E:164:SER:HB3	2.40	0.56
1:C:154:LYS:NZ	1:C:159:LEU:HB2	2.20	0.56
2:D:113:VAL:CA	2:D:114:THR:OG1	2.54	0.56
2:B:15:SER:HA	2:B:84:SER:HA	1.89	0.55
1:C:47:GLY:HA2	1:C:48:GLN:C	2.30	0.55
2:D:24:VAL:HG11	2:D:29:LEU:HD11	1.88	0.55
1:A:96:GLN:O	1:A:101:PRO:HA	2.06	0.55
2:D:201:ASN:CB	2:D:212:ASP:OD1	2.53	0.55
1:E:202:THR:HG23	1:E:209:PRO:HG3	1.89	0.55
2:F:6:GLU:OE1	2:F:110:GLY:N	2.34	0.55
2:B:91:ALA:HB3	2:B:93:TYR:CE1	2.41	0.55
1:E:146:PRO:C	1:E:148:GLU:HG2	2.28	0.55
2:D:158:TRP:O	2:D:160:SER:N	2.39	0.54
1:E:168:VAL:HG12	1:E:180:LEU:HD12	1.88	0.54
1:C:129:GLN:HG2	1:C:134:THR:HG23	1.90	0.54
2:F:130:PRO:C	2:F:218:LYS:HD2	2.31	0.54
2:B:29:LEU:HD12	2:B:29:LEU:H	1.72	0.54
1:A:6:GLN:NE2	1:A:92:TYR:O	2.38	0.54
1:A:160:GLN:NE2	1:A:163:ASN:ND2	2.56	0.53
1:C:81:ILE:HD12	1:C:81:ILE:C	2.32	0.53
1:E:146:PRO:HB2	1:E:148:GLU:OE2	2.09	0.53
2:B:11:LEU:HB2	2:B:151:PRO:HG3	1.90	0.53
1:E:8:PRO:CG	1:E:11:LEU:HG	2.39	0.53
2:D:156:VAL:HA	2:D:202:VAL:H	1.72	0.53
2:D:159:ASN:N	2:D:199:ILE:O	2.25	0.53
2:B:128:LEU:CD1	2:B:145:LEU:HB2	2.38	0.53
1:E:121:PHE:CD2	1:E:140:LEU:HD12	2.39	0.53
2:D:12:VAL:CG2	2:D:85:LEU:HD13	2.39	0.53
1:C:24:LYS:HE3	1:C:24:LYS:N	2.25	0.52
1:C:165:GLN:NE2	2:D:175:GLN:NE2	2.58	0.52
2:F:130:PRO:HG3	2:F:142:LEU:HB3	1.90	0.52
2:D:182:LEU:C	2:D:182:LEU:HD12	2.35	0.52
1:C:130:LEU:C	1:C:132:SER:H	2.18	0.52
2:D:66:ARG:HH22	2:D:89:ASP:CG	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:THR:HA	2:D:115:VAL:HG12	1.92	0.51
2:F:140:ALA:HA	2:F:141:ALA:HB3	1.91	0.51
1:A:117:ALA:HB2	1:A:205:GLY:O	2.11	0.51
1:C:121:PHE:HB2	1:C:140:LEU:HB3	1.92	0.51
1:E:13:VAL:CG1	1:E:84:VAL:HG11	2.40	0.51
1:E:146:PRO:HB2	1:E:148:GLU:CG	2.41	0.51
2:B:35:SER:HA	2:B:50:VAL:HA	1.93	0.51
2:D:111:THR:HA	2:D:112:SER:OG	2.11	0.51
2:B:155:THR:CG2	2:B:203:ASN:O	2.59	0.50
2:F:87:THR:O	2:F:90:THR:CG2	2.45	0.50
2:F:6:GLU:OE2	2:F:108:GLY:HA3	2.11	0.50
2:D:67:LEU:CD1	2:D:82:MET:HG3	2.41	0.50
2:D:199:ILE:O	2:D:199:ILE:HG13	2.12	0.50
2:D:14:PRO:O	2:D:85:LEU:HB2	2.10	0.50
2:F:16:GLN:HG3	2:F:17:SER:H	1.77	0.49
1:E:13:VAL:HG11	1:E:84:VAL:HG11	1.94	0.49
1:E:56:TRP:O	1:E:57:ALA:HB3	2.13	0.49
2:F:207:SER:OG	2:F:209:THR:OG1	2.23	0.49
1:A:41:TRP:CG	1:A:79:LEU:HD13	2.46	0.49
1:C:86:ALA:O	1:C:173:SER:O	2.30	0.49
2:D:195:THR:HG23	2:D:196:GLN:HG2	1.93	0.49
1:A:44:GLN:O	1:A:90:ALA:HB1	2.11	0.49
1:A:45:LYS:O	1:A:48:GLN:HB2	2.12	0.49
2:D:24:VAL:HG21	2:D:27:PHE:CZ	2.48	0.49
1:A:160:GLN:HE21	1:A:163:ASN:HD21	1.61	0.48
2:D:125:VAL:O	2:D:213:LYS:HE3	2.12	0.48
2:D:205:LYS:HB3	2:D:206:PRO:HD3	1.95	0.48
2:F:149:TYR:CE2	2:F:154:VAL:HG23	2.48	0.48
2:B:205:LYS:HB2	2:B:206:PRO:HD3	1.95	0.48
1:E:163:ASN:OD1	1:E:163:ASN:N	2.44	0.48
2:F:140:ALA:CA	2:F:141:ALA:CB	2.91	0.48
2:F:72:ASP:OD1	2:F:74:SER:OG	2.30	0.48
2:D:196:GLN:HB3	2:D:198:TYR:CZ	2.49	0.48
2:D:199:ILE:CA	2:D:200:CYS:CB	2.90	0.48
2:D:42:GLY:O	2:D:43:LYS:HD2	2.13	0.48
2:F:172:ALA:HA	2:F:182:LEU:HB3	1.96	0.48
1:A:46:PRO:CG	1:A:170:GLU:HG2	2.42	0.48
1:A:86:ALA:HA	1:A:111:LEU:HG	1.95	0.48
2:D:22:CYS:HB3	2:D:78:VAL:CG1	2.29	0.47
1:E:147:ARG:H	1:E:148:GLU:CG	2.22	0.47
2:F:14:PRO:C	2:F:16:GLN:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:PRO:HG3	2:B:142:LEU:HB3	1.96	0.47
1:A:13:VAL:HG11	1:A:84:VAL:HG11	1.96	0.47
1:C:8:PRO:HG2	1:C:11:LEU:HG	1.96	0.47
2:F:140:ALA:CA	2:F:141:ALA:HB3	2.44	0.47
1:A:11:LEU:HD13	1:A:19:VAL:HG21	1.96	0.47
1:E:156:ASP:HA	1:E:196:VAL:HB	1.96	0.47
2:B:182:LEU:C	2:B:182:LEU:HD12	2.40	0.47
1:C:129:GLN:O	1:C:132:SER:HB3	2.15	0.47
2:D:26:GLY:O	2:D:27:PHE:HB3	2.14	0.47
2:D:59:TYR:CE1	2:D:69:ILE:HG13	2.50	0.47
2:F:120:THR:HG22	2:F:207:SER:HB3	1.95	0.47
1:A:67:ARG:HD2	1:A:83:SER:O	2.15	0.47
2:D:39:GLN:C	2:D:91:ALA:HB1	2.40	0.46
2:B:29:LEU:HD12	2:B:29:LEU:N	2.30	0.46
1:C:118:PRO:HA	1:C:144:PHE:HB3	1.97	0.46
1:C:126:SER:CB	2:D:126:PHE:HE1	2.29	0.46
1:C:164:SER:HA	1:C:183:THR:O	2.15	0.46
1:C:165:GLN:NE2	2:D:175:GLN:HE22	2.13	0.46
1:E:25:SER:O	1:E:75:THR:HG23	2.15	0.46
1:E:28:SER:HA	1:E:74:GLY:O	2.15	0.46
2:D:163:LEU:HD21	2:D:186:VAL:CG2	2.32	0.46
1:E:190:ASP:O	1:E:193:LYS:HB3	2.15	0.46
1:A:48:GLN:HA	1:A:49:SER:CB	2.45	0.46
2:D:63:LEU:O	2:D:64:LYS:C	2.58	0.46
2:D:148:ASP:HB2	2:D:179:LEU:HD13	1.98	0.46
1:C:140:LEU:HD22	2:D:185:VAL:HG21	1.97	0.46
1:C:22:SER:HB2	1:C:24:LYS:HE2	1.98	0.46
1:E:145:TYR:CG	1:E:146:PRO:HA	2.51	0.46
2:D:33:GLY:HA3	2:D:52:TRP:HE3	1.81	0.46
1:E:174:LYS:HG2	1:E:175:ASP:H	1.81	0.46
1:C:146:PRO:HB2	1:C:148:GLU:OE1	2.15	0.45
1:A:160:GLN:CB	1:A:163:ASN:HD21	2.23	0.45
1:E:12:ALA:HB1	1:E:112:LYS:HG3	1.98	0.45
1:C:39:LEU:HD13	1:C:39:LEU:C	2.41	0.45
2:D:27:PHE:CE2	2:D:97:LYS:HE3	2.51	0.45
1:C:123:PHE:O	1:C:137:VAL:HG23	2.16	0.45
2:F:90:THR:CG2	2:F:115:VAL:H	2.28	0.45
1:C:175:ASP:O	1:C:176:SER:HB2	2.16	0.45
1:A:29:LEU:HD23	1:A:39:LEU:HB2	1.98	0.45
1:C:202:THR:CG2	1:C:209:PRO:HG3	2.39	0.45
1:E:150:LYS:O	1:E:201:VAL:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLN:NE2	1:A:163:ASN:HD21	2.15	0.45
1:A:15:ALA:O	1:A:84:VAL:O	2.35	0.45
2:D:93:TYR:N	2:D:111:THR:O	2.48	0.45
1:C:121:PHE:CD2	2:D:141:ALA:HB3	2.52	0.44
2:D:86:GLN:C	2:D:115:VAL:HG11	2.41	0.44
2:D:87:THR:HA	2:D:115:VAL:HG11	1.99	0.44
2:D:126:PHE:CD1	2:D:127:PRO:HD2	2.51	0.44
1:E:118:PRO:HA	1:E:144:PHE:HB3	2.00	0.44
2:B:130:PRO:HD2	2:B:217:PRO:HA	1.99	0.44
1:C:17:GLU:O	1:C:84:VAL:HG12	2.18	0.44
1:C:202:THR:HG22	1:C:209:PRO:CG	2.39	0.44
2:D:143:GLY:HA2	2:D:158:TRP:CH2	2.52	0.44
2:D:22:CYS:O	2:D:77:GLN:HA	2.18	0.44
1:C:45:LYS:HE2	1:C:87:GLU:O	2.17	0.44
1:E:118:PRO:CA	1:E:144:PHE:HB3	2.48	0.44
2:D:66:ARG:NH1	2:D:83:ASN:O	2.49	0.44
1:A:84:VAL:HG23	1:A:88:ASP:HB2	2.00	0.43
1:C:130:LEU:C	1:C:132:SER:N	2.76	0.43
1:E:34:THR:HG21	1:E:38:TYR:OH	2.18	0.43
2:F:182:LEU:C	2:F:182:LEU:HD12	2.42	0.43
2:B:214:LYS:H	2:B:214:LYS:HG2	1.48	0.43
1:A:197:TYR:O	1:A:213:SER:HA	2.18	0.43
1:E:4:MET:CE	1:E:96:GLN:CB	2.88	0.43
1:E:4:MET:HE1	1:E:29:LEU:HD21	2.01	0.43
1:E:31:ASN:HB2	1:E:38:TYR:HE2	1.83	0.43
2:F:140:ALA:HA	2:F:141:ALA:HB2	1.99	0.43
1:C:129:GLN:HB2	2:D:126:PHE:CD1	2.53	0.43
2:D:201:ASN:HA	2:D:202:VAL:CB	2.48	0.43
1:C:4:MET:HE3	1:C:23:CYS:SG	2.59	0.43
1:E:174:LYS:CG	1:E:175:ASP:N	2.82	0.43
2:F:47:TRP:CH2	2:F:49:GLY:HA2	2.53	0.43
1:E:60:ARG:NH2	1:E:66:ASP:O	2.50	0.43
2:F:5:LYS:O	2:F:22:CYS:HA	2.18	0.43
1:C:101:PRO:HD2	2:D:47:TRP:CH2	2.53	0.43
2:F:129:ALA:HA	2:F:130:PRO:HD3	1.72	0.43
2:D:192:SER:HB2	2:D:196:GLN:HG3	2.00	0.42
1:E:44:GLN:HB2	1:E:50:PRO:HB3	2.01	0.42
1:A:41:TRP:CE2	1:A:79:LEU:HB2	2.54	0.42
1:C:68:PHE:HD1	1:C:81:ILE:HG22	1.81	0.42
1:E:100:LEU:HA	1:E:101:PRO:HD3	1.67	0.42
1:E:175:ASP:OD1	1:E:175:ASP:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PRO:HG2	2:B:107:TRP:CZ3	2.54	0.42
1:C:19:VAL:CG2	1:C:81:ILE:CD1	2.97	0.42
1:C:139:CYS:HB2	1:C:153:TRP:CH2	2.55	0.42
1:E:147:ARG:NH2	1:E:168:VAL:HG21	2.34	0.42
2:B:152:GLU:HA	2:B:153:PRO:HA	1.76	0.42
1:E:14:SER:HB2	1:E:17:GLU:HG3	2.02	0.42
1:E:168:VAL:HG13	1:E:180:LEU:HD12	2.01	0.42
2:D:59:TYR:HE1	2:D:69:ILE:HG13	1.84	0.41
2:D:161:GLY:O	2:D:164:THR:HG23	2.20	0.41
1:E:53:LEU:C	1:E:54:ILE:HG12	2.44	0.41
1:C:19:VAL:HG23	1:C:81:ILE:CD1	2.49	0.41
2:B:38:ARG:NH1	2:B:82:MET:HE1	2.35	0.41
1:C:86:ALA:HA	1:C:111:LEU:HG	2.03	0.41
1:C:156:ASP:OD2	1:C:194:HIS:HB3	2.21	0.41
2:B:170:PHE:HD1	2:B:183:SER:O	2.02	0.41
1:E:7:SER:HA	1:E:8:PRO:C	2.46	0.41
2:F:48:LEU:HD23	2:F:48:LEU:HA	1.82	0.41
1:A:36:LYS:HE3	1:A:56:TRP:CE3	2.56	0.41
1:C:89:LEU:O	1:C:90:ALA:HB2	2.20	0.41
2:D:11:LEU:HD23	2:D:120:THR:HG22	2.03	0.41
2:D:27:PHE:HD1	2:D:28:SER:O	2.03	0.41
1:E:45:LYS:HE2	1:E:87:GLU:O	2.21	0.41
2:F:121:LYS:NZ	3:F:304:HOH:O	2.51	0.41
2:B:129:ALA:HA	2:B:130:PRO:HD3	1.91	0.41
1:C:139:CYS:HB2	1:C:153:TRP:CZ2	2.55	0.41
2:D:29:LEU:N	2:D:73:ASN:OD1	2.48	0.41
2:D:39:GLN:HB2	2:D:45:LEU:HD23	2.03	0.41
2:D:104:GLY:CA	2:D:105:ASP:CB	2.70	0.41
1:E:146:PRO:HB2	1:E:148:GLU:HG3	2.02	0.41
1:A:129:GLN:HG2	1:A:134:THR:HG23	2.03	0.41
2:F:128:LEU:HB2	2:F:143:GLY:C	2.46	0.41
1:C:45:LYS:O	1:C:46:PRO:C	2.64	0.40
1:E:67:ARG:NH2	1:E:85:GLN:CG	2.83	0.40
1:A:36:LYS:HD2	1:A:56:TRP:CG	2.56	0.40
2:D:53:GLY:O	2:D:71:LYS:NZ	2.52	0.40
2:F:59:TYR:HD2	2:F:67:LEU:HD23	1.87	0.40
1:C:137:VAL:CG1	1:C:184:LEU:HB3	2.49	0.40
1:E:29:LEU:O	1:E:37:ASN:HA	2.21	0.40
1:C:190:ASP:O	1:C:193:LYS:HB3	2.21	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	206/219 (94%)	188 (91%)	15 (7%)	3 (2%)	8	16
1	C	209/219 (95%)	193 (92%)	11 (5%)	5 (2%)	4	8
1	E	212/219 (97%)	186 (88%)	18 (8%)	8 (4%)	2	3
2	B	202/238 (85%)	179 (89%)	16 (8%)	7 (4%)	3	4
2	D	206/238 (87%)	176 (85%)	16 (8%)	14 (7%)	1	1
2	F	201/238 (84%)	184 (92%)	13 (6%)	4 (2%)	6	11
All	All	1236/1371 (90%)	1106 (90%)	89 (7%)	41 (3%)	3	4

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	148	GLU
2	B	105	ASP
2	B	153	PRO
2	B	162	ALA
1	C	48	GLN
2	D	100	TYR
2	D	105	ASP
2	D	113	VAL
2	D	148	ASP
2	D	200	CYS
1	E	148	GLU
2	F	98	HIS
2	F	141	ALA
2	B	148	ASP
2	D	56	SER
2	D	159	ASN
1	E	26	SER
2	B	56	SER
2	B	155	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	48	GLN
1	E	156	ASP
1	E	161	SER
1	C	74	GLY
1	C	131	LYS
2	D	14	PRO
2	D	153	PRO
1	E	49	SER
1	E	99	ASP
1	E	204	GLN
2	F	148	ASP
1	A	143	ASN
1	C	47	GLY
2	D	27	PHE
2	D	112	SER
2	D	202	VAL
2	B	104	GLY
2	D	114	THR
2	D	9	PRO
1	C	49	SER
2	F	153	PRO

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	185/193 (96%)	170 (92%)	15 (8%)	11	23
1	C	187/193 (97%)	172 (92%)	15 (8%)	11	24
1	E	188/193 (97%)	171 (91%)	17 (9%)	9	19
2	B	176/205 (86%)	156 (89%)	20 (11%)	5	11
2	D	176/205 (86%)	165 (94%)	11 (6%)	16	34
2	F	176/205 (86%)	158 (90%)	18 (10%)	7	14
All	All	1088/1194 (91%)	992 (91%)	96 (9%)	9	20

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	39	LEU
1	A	49	SER
1	A	51	THR
1	A	53	LEU
1	A	59	THR
1	A	76	ASP
1	A	78	THR
1	A	81	ILE
1	A	97	SER
1	A	100	LEU
1	A	112	LYS
1	A	148	GLU
1	A	190	ASP
1	A	213	SER
2	B	5	LYS
2	B	17	SER
2	B	56	SER
2	B	78	VAL
2	B	84	SER
2	B	86	GLN
2	B	97	LYS
2	B	116	SER
2	B	128	LEU
2	B	139	THR
2	B	142	LEU
2	B	148	ASP
2	B	160	SER
2	B	163	LEU
2	B	181	SER
2	B	183	SER
2	B	190	SER
2	B	191	SER
2	B	201	ASN
2	B	209	THR
1	C	2	ILE
1	C	5	SER
1	C	13	VAL
1	C	19	VAL
1	C	24	LYS
1	C	53	LEU
1	C	54	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	66	ASP
1	C	75	THR
1	C	82	SER
1	C	84	VAL
1	C	100	LEU
1	C	126	SER
1	C	151	VAL
1	C	210	VAL
2	D	15	SER
2	D	17	SER
2	D	23	THR
2	D	65	SER
2	D	97	LYS
2	D	142	LEU
2	D	144	CYS
2	D	146	VAL
2	D	148	ASP
2	D	190	SER
2	D	211	VAL
1	E	9	SER
1	E	13	VAL
1	E	32	SER
1	E	48	GLN
1	E	51	THR
1	E	53	LEU
1	E	54	ILE
1	E	80	THR
1	E	84	VAL
1	E	89	LEU
1	E	96	GLN
1	E	119	SER
1	E	128	GLU
1	E	148	GLU
1	E	165	GLN
1	E	202	THR
1	E	206	LEU
2	F	24	VAL
2	F	29	LEU
2	F	30	THR
2	F	56	SER
2	F	68	SER
2	F	76	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	84	SER
2	F	90	THR
2	F	97	LYS
2	F	98	HIS
2	F	99	THR
2	F	139	THR
2	F	148	ASP
2	F	163	LEU
2	F	183	SER
2	F	190	SER
2	F	201	ASN
2	F	216	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	143	ASN
1	A	152	GLN
1	A	160	GLN
1	A	163	ASN
1	A	165	GLN
2	B	159	ASN
2	B	168	HIS
2	B	175	GLN
2	B	201	ASN
1	C	165	GLN
1	C	194	HIS
1	C	204	GLN
2	D	86	GLN
2	D	168	HIS
2	D	175	GLN
1	E	96	GLN
1	E	143	ASN
1	E	160	GLN
1	E	194	HIS
2	F	203	ASN

5.3.3 RNA ⓘ

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 [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	210/219 (95%)	0.06	1 (0%) 87 86	37, 66, 89, 110	0
1	C	213/219 (97%)	0.04	1 (0%) 87 86	34, 59, 89, 112	0
1	E	214/219 (97%)	0.04	2 (0%) 81 79	31, 59, 95, 127	0
2	B	208/238 (87%)	0.18	0 100 100	37, 67, 97, 113	0
2	D	210/238 (88%)	0.56	6 (2%) 53 49	49, 85, 116, 131	0
2	F	207/238 (86%)	0.04	5 (2%) 59 55	35, 57, 84, 127	0
All	All	1262/1371 (92%)	0.15	15 (1%) 76 74	31, 65, 101, 131	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	141	ALA	3.9
2	F	52	TRP	3.8
2	D	98	HIS	2.8
1	A	31	ASN	2.7
2	F	105	ASP	2.6
1	E	47	GLY	2.6
2	D	2	VAL	2.5
2	F	106	SER	2.4
2	D	101	GLY	2.3
2	F	218	LYS	2.3
2	D	195	THR	2.2
1	E	148	GLU	2.2
2	D	100	TYR	2.2
1	C	216	ARG	2.2
2	D	99	THR	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.