



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:59 PM UTC

PDB ID : 3ZRF / pdb_00003zrf
Title : pVHL54-213-EloB-EloC complex_apo
Authors : Van Molle, I.; Buckley, D.L.; Crews, C.M.; Ciulli, A.
Deposited on : 2011-06-16
Resolution : 2.80 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:

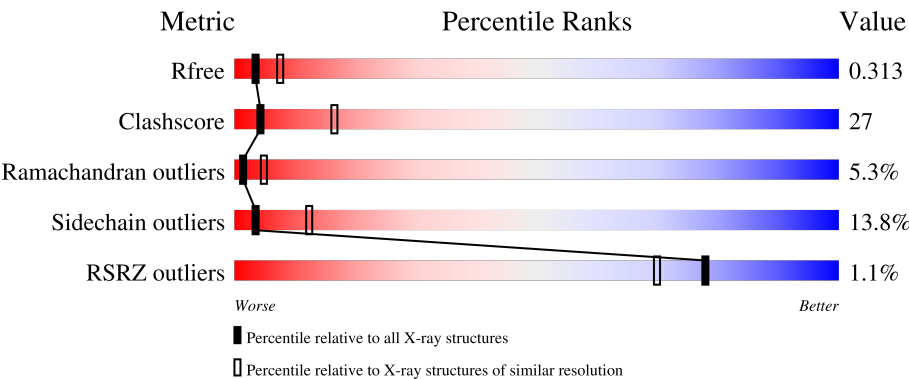
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	118	4% 47%29%9%14%
1	D	118	3% 42%28%13%17%
1	G	118	2% 32%47%8%11%
1	J	118	38%38%12%11%
2	B	97	43%33%12%11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	97	37%45%5%10%
2	H	97	33%43%12%11%
2	K	97	% 32%43%12%12%
3	C	163	% 40%35%9%13%
3	F	163	43%34%8%13%
3	I	163	36%42%7%11%
3	L	163	% 37%38%11%12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10354 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 TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			768	490	127	147	4			
1	D	98	Total	C	N	O	S	0	0	0
			719	457	119	139	4			
1	G	105	Total	C	N	O	S	0	0	0
			809	512	136	156	5			
1	J	105	Total	C	N	O	S	0	0	0
			822	520	139	158	5			

- Molecule 2 is a protein called TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			666	431	105	124	6			
2	E	87	Total	C	N	O	S	0	0	0
			680	440	107	127	6			
2	H	86	Total	C	N	O	S	0	0	0
			683	442	109	126	6			
2	K	85	Total	C	N	O	S	0	0	0
			678	439	108	125	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15369
E	16	MET	-	expression tag	UNP Q15369
H	16	MET	-	expression tag	UNP Q15369
K	16	MET	-	expression tag	UNP Q15369

- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	142	Total	C	N	O	S	0	0	0
			1058	675	188	193	2			
3	F	142	Total	C	N	O	S	0	0	0
			1115	710	198	205	2			
3	I	145	Total	C	N	O	S	0	0	0
			1164	741	211	210	2			
3	L	143	Total	C	N	O	S	0	0	0
			1143	730	207	204	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	51	GLY	-	expression tag	UNP P40337
C	52	SER	-	expression tag	UNP P40337
C	53	HIS	-	expression tag	UNP P40337
F	51	GLY	-	expression tag	UNP P40337
F	52	SER	-	expression tag	UNP P40337
F	53	HIS	-	expression tag	UNP P40337
I	51	GLY	-	expression tag	UNP P40337
I	52	SER	-	expression tag	UNP P40337
I	53	HIS	-	expression tag	UNP P40337
L	51	GLY	-	expression tag	UNP P40337
L	52	SER	-	expression tag	UNP P40337
L	53	HIS	-	expression tag	UNP P40337

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	C	4	Total	O	0	0
			4	4		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		
4	F	6	Total	O	0	0
			6	6		
4	G	7	Total	O	0	0
			7	7		
4	H	4	Total	O	0	0
			4	4		
4	I	5	Total	O	0	0
			5	5		

Continued on next page...

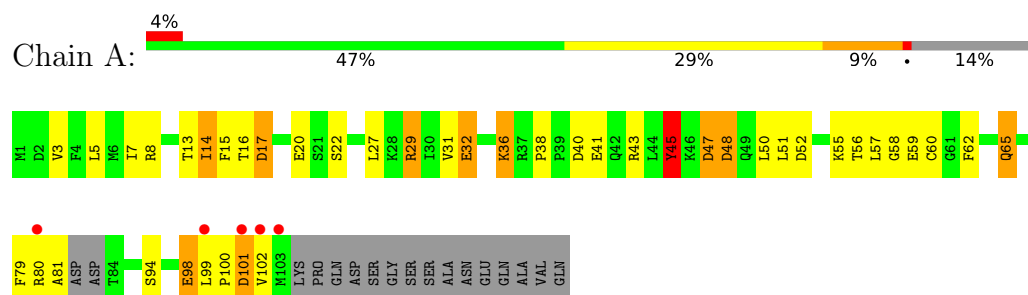
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	3	Total 3	O 3	0	0
4	K	5	Total 5	O 5	0	0
4	L	9	Total 9	O 9	0	0

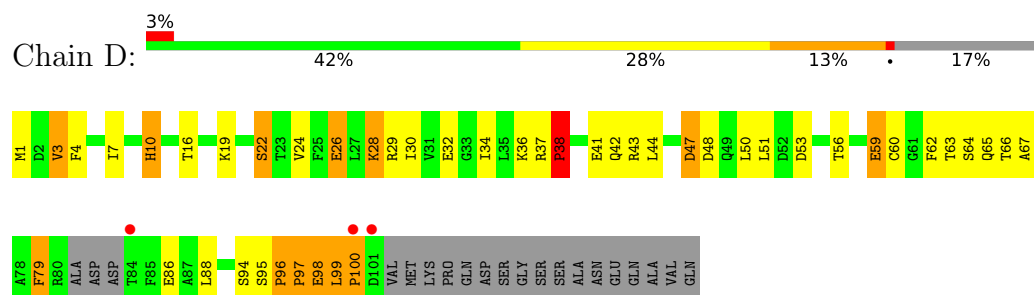
3 Residue-property plots [i](#)

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.

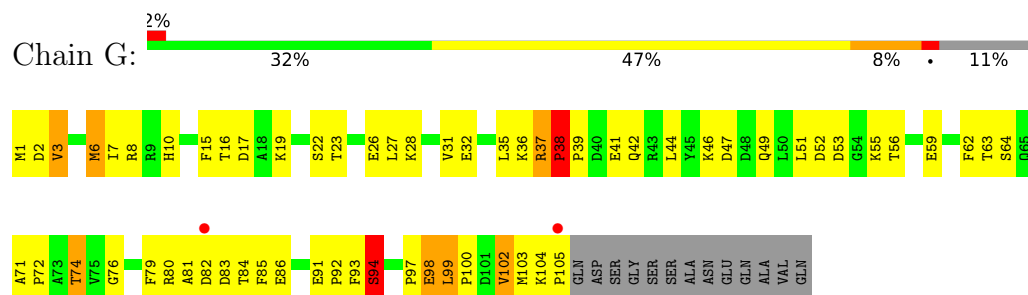
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



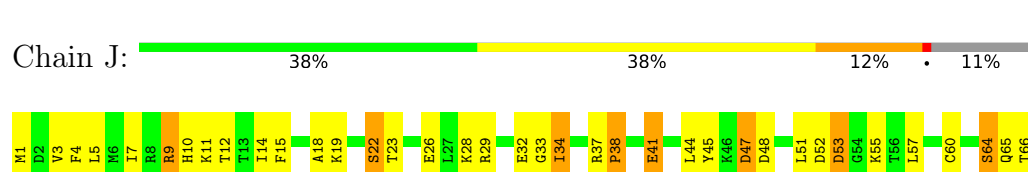
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

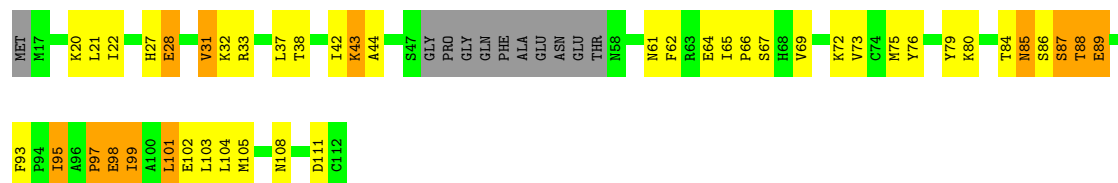


• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

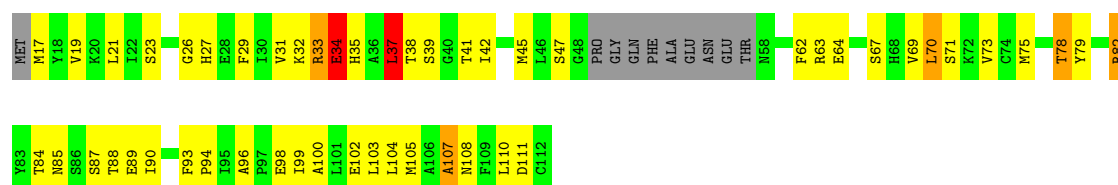




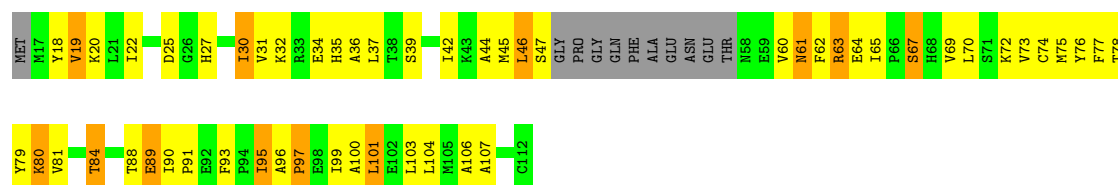
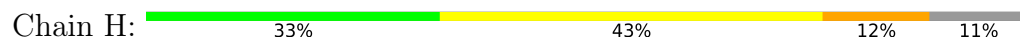
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



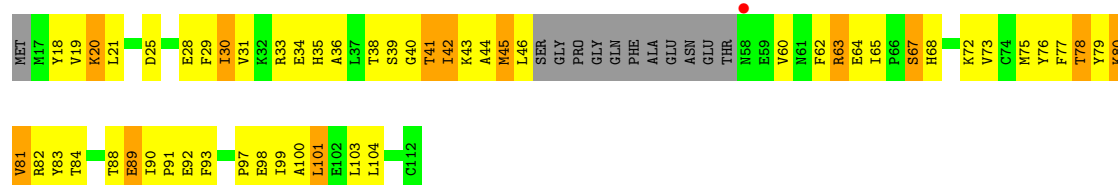
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

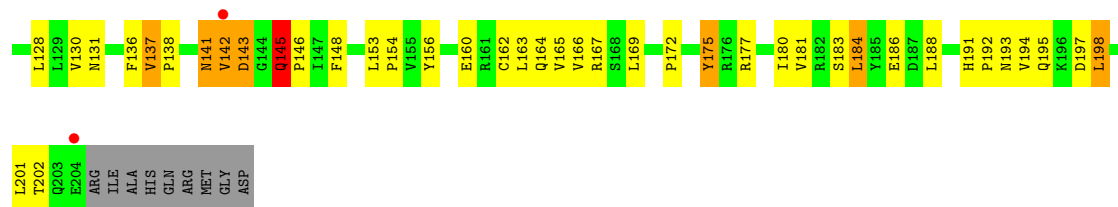


• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



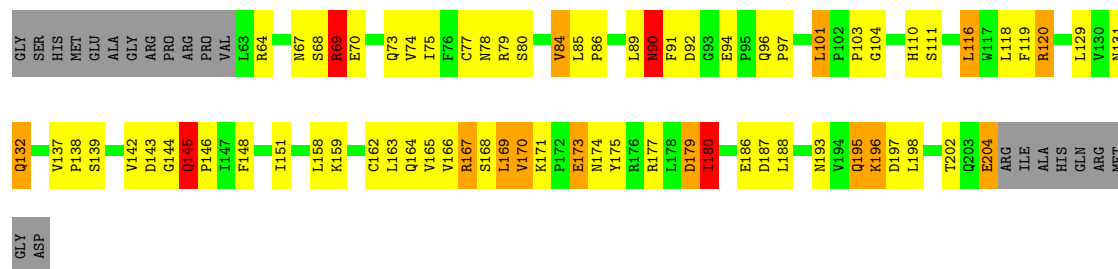
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,





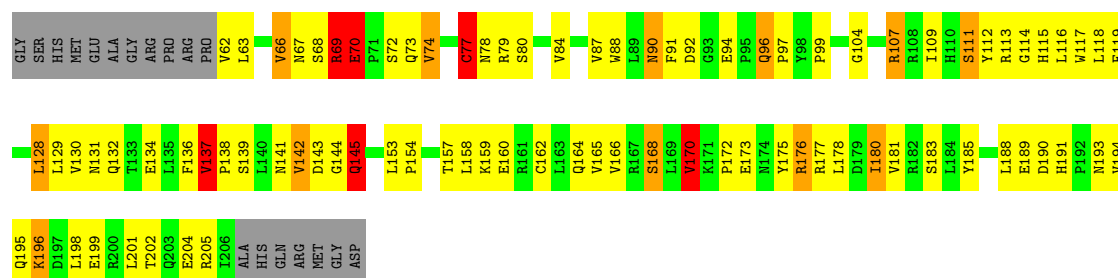
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,

Chain F: 43% 34% 8% • 13%



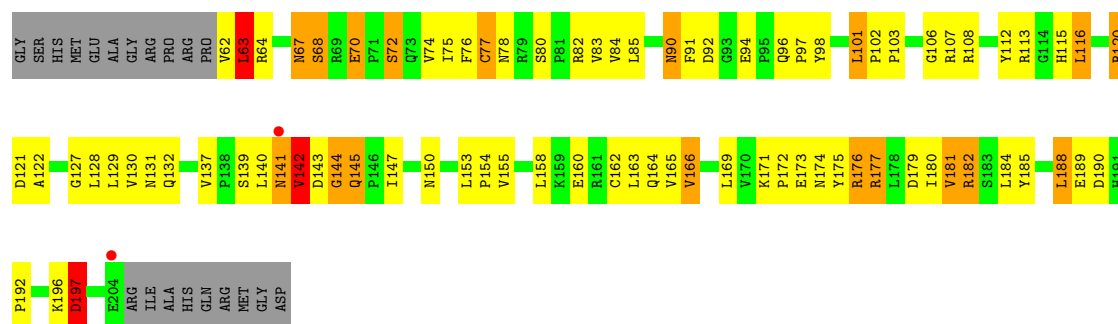
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,

Chain I: 36% 42% 7% • 11%



• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR,

Chain L: 37% 38% 11% • 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.08Å 93.08Å 364.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 2.80 46.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.54-2.80) 99.5 (46.54-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.320 0.219 , 0.313	Depositor DCC
R_{free} test set	2027 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10354	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5400e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.37	2/783 (0.3%)	1.56	11/1061 (1.0%)
1	D	1.25	2/733 (0.3%)	1.43	7/997 (0.7%)
1	G	1.14	0/826	1.37	7/1120 (0.6%)
1	J	1.39	5/839 (0.6%)	1.48	7/1135 (0.6%)
2	B	1.32	3/680 (0.4%)	1.54	10/920 (1.1%)
2	E	1.32	2/694 (0.3%)	1.42	7/936 (0.7%)
2	H	1.21	1/697 (0.1%)	1.45	11/940 (1.2%)
2	K	1.41	4/692 (0.6%)	1.48	6/933 (0.6%)
3	C	1.22	2/1086 (0.2%)	1.47	18/1493 (1.2%)
3	F	1.29	5/1144 (0.4%)	1.38	8/1566 (0.5%)
3	I	1.26	6/1194 (0.5%)	1.43	18/1631 (1.1%)
3	L	1.33	5/1173 (0.4%)	1.60	16/1603 (1.0%)
All	All	1.29	37/10541 (0.4%)	1.47	126/14335 (0.9%)

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	G	0	1
1	J	0	1
3	C	0	1
3	F	0	1
3	L	0	2
All	All	0	6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	75	VAL	CA-CB	8.86	1.64	1.54
3	F	145	GLN	CA-C	7.47	1.62	1.52
3	I	77	CYS	CB-SG	7.34	2.05	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	GLU	N-CA	7.06	1.50	1.46
2	B	66	PRO	CA-C	6.99	1.60	1.52
3	L	83	VAL	CA-CB	-6.81	1.45	1.54
3	F	84	VAL	CA-CB	6.72	1.61	1.54
1	J	38	PRO	CA-C	6.43	1.56	1.52
2	B	108	ASN	CA-C	6.32	1.60	1.52
3	L	77	CYS	CA-CB	6.11	1.61	1.53
2	K	88	THR	CA-C	5.91	1.59	1.53
2	E	107	ALA	CA-CB	5.90	1.62	1.53
2	K	101	LEU	CA-C	-5.89	1.45	1.52
3	F	80	SER	CA-C	-5.80	1.46	1.52
2	B	27	HIS	CA-C	-5.77	1.45	1.52
3	I	128	LEU	CA-C	-5.76	1.45	1.52
3	I	153	LEU	CA-C	-5.63	1.45	1.53
3	L	101	LEU	C-O	-5.56	1.20	1.25
3	F	85	LEU	C-O	-5.55	1.20	1.25
1	J	91	GLU	CA-C	-5.52	1.46	1.53
1	A	16	THR	N-CA	-5.46	1.39	1.45
1	D	79	PHE	CA-C	5.44	1.59	1.52
3	L	171	LYS	N-CA	5.40	1.52	1.45
3	F	180	ILE	CA-CB	5.36	1.61	1.54
3	L	166	VAL	N-CA	-5.36	1.40	1.46
2	K	30	ILE	CA-CB	5.31	1.61	1.54
1	J	73	ALA	CA-CB	-5.29	1.44	1.53
3	C	64	ARG	CA-C	5.20	1.59	1.52
2	H	106	ALA	CA-CB	-5.15	1.45	1.53
3	I	128	LEU	C-O	-5.10	1.17	1.23
3	I	69	ARG	N-CA	-5.09	1.40	1.46
1	J	9	ARG	CA-C	-5.09	1.46	1.52
2	E	90	ILE	CA-C	5.08	1.58	1.52
1	A	14	ILE	CA-CB	5.03	1.60	1.54
3	C	66	VAL	CA-C	5.02	1.58	1.52
2	K	92	GLU	N-CA	-5.02	1.39	1.46
3	I	77	CYS	CA-CB	5.01	1.60	1.53

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	98	TYR	CA-C-N	-12.22	107.93	120.03
3	L	98	TYR	C-N-CA	-12.22	107.93	120.03
1	G	37	ARG	CA-C-N	9.96	130.63	120.38
1	G	37	ARG	C-N-CA	9.96	130.63	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	143	ASP	N-CA-C	-9.79	98.22	111.54
3	C	102	PRO	CA-C-N	9.78	132.07	119.84
3	C	102	PRO	C-N-CA	9.78	132.07	119.84
3	I	159	LYS	N-CA-C	-9.49	100.92	111.07
3	C	175	TYR	N-CA-C	8.81	122.04	111.82
3	L	80	SER	N-CA-C	-8.65	100.43	108.22
1	D	96	PRO	CA-C-N	8.37	130.31	119.84
1	D	96	PRO	C-N-CA	8.37	130.31	119.84
1	D	37	ARG	CA-C-N	8.22	128.84	120.38
1	D	37	ARG	C-N-CA	8.22	128.84	120.38
3	C	153	LEU	CA-C-N	-8.16	112.03	120.85
3	C	153	LEU	C-N-CA	-8.16	112.03	120.85
1	J	91	GLU	CA-C-N	8.15	128.64	119.92
1	J	91	GLU	C-N-CA	8.15	128.64	119.92
3	I	91	PHE	N-CA-C	-8.05	102.56	112.38
3	C	75	ILE	N-CA-C	7.92	119.73	108.17
2	H	44	ALA	N-CA-C	-7.82	102.44	110.97
3	I	145	GLN	CA-C-N	-7.80	110.08	119.84
3	I	145	GLN	C-N-CA	-7.80	110.08	119.84
2	H	65	ILE	N-CA-C	7.78	116.60	107.73
3	F	101	LEU	CA-C-N	-7.73	112.41	120.38
3	F	101	LEU	C-N-CA	-7.73	112.41	120.38
2	H	61	ASN	N-CA-C	7.67	123.11	107.69
2	B	21	LEU	CA-C-N	-7.58	113.79	123.19
2	B	21	LEU	C-N-CA	-7.58	113.79	123.19
1	D	79	PHE	N-CA-C	7.44	121.63	109.72
2	B	27	HIS	N-CA-C	7.33	120.61	110.35
3	L	145	GLN	N-CA-C	7.24	119.85	108.55
3	I	70	GLU	CA-C-N	-7.09	111.57	120.51
3	I	70	GLU	C-N-CA	-7.09	111.57	120.51
2	H	93	PHE	CA-C-N	-6.92	112.81	120.14
2	H	93	PHE	C-N-CA	-6.92	112.81	120.14
2	K	18	TYR	N-CA-C	6.84	119.57	109.24
3	L	68	SER	N-CA-C	-6.74	100.50	110.48
1	A	65	GLN	N-CA-C	-6.73	103.41	111.69
1	G	98	GLU	CA-C-N	6.67	133.70	121.70
1	G	98	GLU	C-N-CA	6.67	133.70	121.70
2	E	34	GLU	N-CA-C	-6.64	103.96	111.14
3	C	165	VAL	N-CA-C	-6.55	104.37	110.53
2	B	99	ILE	N-CA-CB	-6.54	103.32	112.35
3	L	137	VAL	CA-C-N	6.52	126.91	119.93
3	L	137	VAL	C-N-CA	6.52	126.91	119.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	47	ASP	CB-CA-C	-6.50	103.15	111.86
1	G	38	PRO	N-CA-C	6.40	118.51	110.70
2	K	88	THR	N-CA-C	6.40	119.57	109.39
3	L	68	SER	CA-C-N	-6.31	112.18	122.65
3	L	68	SER	C-N-CA	-6.31	112.18	122.65
2	B	75	MET	N-CA-C	-6.26	104.53	111.36
3	I	68	SER	CA-C-N	-6.23	112.50	122.66
3	I	68	SER	C-N-CA	-6.23	112.50	122.66
1	A	79	PHE	N-CA-C	6.14	119.66	110.14
2	H	65	ILE	CA-C-N	-6.13	114.33	120.21
2	H	65	ILE	C-N-CA	-6.13	114.33	120.21
1	A	52	ASP	CB-CA-C	-6.12	100.00	110.22
2	E	90	ILE	CA-C-N	6.11	126.61	120.14
2	E	90	ILE	C-N-CA	6.11	126.61	120.14
3	I	170	VAL	N-CA-C	6.09	117.54	108.46
1	J	91	GLU	N-CA-C	-6.02	102.46	109.93
2	E	64	GLU	N-CA-C	5.98	121.50	113.72
3	C	74	VAL	CA-C-N	-5.98	114.08	122.75
3	C	74	VAL	C-N-CA	-5.98	114.08	122.75
2	B	111	ASP	CB-CA-C	-5.96	104.19	111.82
3	I	137	VAL	CA-C-N	5.87	127.17	119.84
3	I	137	VAL	C-N-CA	5.87	127.17	119.84
3	L	67	ASN	N-CA-C	5.86	119.79	110.70
2	K	104	LEU	N-CA-C	-5.84	104.83	111.14
1	A	52	ASP	N-CA-C	5.83	118.23	108.96
1	D	38	PRO	N-CA-C	5.83	117.82	110.70
1	D	10	HIS	N-CA-C	5.80	123.16	110.80
1	J	90	ILE	CB-CA-C	-5.80	102.05	110.63
2	E	26	GLY	N-CA-C	5.75	121.54	114.69
2	E	82	ARG	N-CA-C	-5.71	106.45	113.41
1	A	55	LYS	N-CA-C	5.70	118.24	110.55
1	A	47	ASP	CB-CA-C	-5.69	103.65	111.73
3	F	94	GLU	CA-C-N	-5.69	113.93	119.90
3	F	94	GLU	C-N-CA	-5.69	113.93	119.90
1	A	38	PRO	O-C-N	5.66	123.81	121.15
3	C	80	SER	CA-C-N	-5.66	112.77	119.84
3	C	80	SER	C-N-CA	-5.66	112.77	119.84
2	B	27	HIS	CB-CA-C	-5.63	100.72	109.61
3	C	169	LEU	N-CA-C	-5.61	107.07	114.31
2	B	86	SER	N-CA-C	5.61	117.38	107.61
2	K	81	VAL	N-CA-C	-5.52	104.94	113.16
3	I	180	ILE	N-CA-C	5.51	116.67	108.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	96	GLN	CA-C-N	5.48	125.65	119.90
3	C	96	GLN	C-N-CA	5.48	125.65	119.90
2	K	33	ARG	N-CA-C	-5.48	105.22	111.14
3	L	197	ASP	N-CA-CB	5.47	118.26	110.16
2	H	67	SER	CB-CA-C	-5.44	102.10	110.81
3	I	77	CYS	N-CA-CB	5.44	119.09	110.55
3	F	137	VAL	N-CA-C	5.43	113.53	108.15
2	H	95	ILE	CB-CA-C	-5.42	102.41	111.29
3	F	129	LEU	CA-C-N	-5.38	115.51	122.99
3	F	129	LEU	C-N-CA	-5.38	115.51	122.99
2	B	101	LEU	CA-CB-CG	-5.38	97.49	116.30
3	L	70	GLU	CA-C-N	-5.34	114.74	120.03
3	L	70	GLU	C-N-CA	-5.34	114.74	120.03
3	I	96	GLN	CA-C-N	5.32	125.24	119.76
3	I	96	GLN	C-N-CA	5.32	125.24	119.76
1	G	2	ASP	N-CA-C	5.29	117.90	109.96
3	C	165	VAL	CB-CA-C	-5.29	105.09	112.02
3	C	64	ARG	N-CA-C	5.29	117.71	109.52
1	J	45	TYR	N-CA-C	5.29	118.02	109.40
3	I	168	SER	N-CA-C	-5.26	106.36	112.89
1	A	71	ALA	CA-C-N	5.25	125.01	119.76
1	A	71	ALA	C-N-CA	5.25	125.01	119.76
2	H	69	VAL	N-CA-C	-5.24	107.66	111.90
2	B	64	GLU	N-CA-C	5.23	120.31	112.94
3	L	153	LEU	CA-C-N	-5.20	115.41	120.98
3	L	153	LEU	C-N-CA	-5.20	115.41	120.98
2	H	106	ALA	N-CA-C	-5.20	105.69	111.36
1	A	45	TYR	N-CA-C	5.18	118.01	109.72
3	I	107	ARG	N-CA-C	5.17	116.46	107.93
3	C	101	LEU	CA-C-N	-5.15	115.08	120.38
3	C	101	LEU	C-N-CA	-5.15	115.08	120.38
1	J	34	ILE	N-CA-C	5.12	116.53	111.67
1	G	47	ASP	CB-CA-C	-5.11	104.64	112.11
3	F	145	GLN	N-CA-C	5.09	121.07	109.81
3	I	142	VAL	N-CA-C	5.08	115.28	108.17
2	E	96	ALA	N-CA-C	-5.06	103.40	109.83
2	K	39	SER	N-CA-C	-5.06	101.72	109.76
1	A	17	ASP	N-CA-C	-5.00	102.79	110.14

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	145	GLN	Peptide
3	F	145	GLN	Peptide
1	G	41	GLU	Peptide
1	J	83	ASP	Peptide
3	L	142	VAL	Peptide
3	L	144	GLY	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	768	0	752	31	0
1	D	719	0	676	35	0
1	G	809	0	787	65	0
1	J	822	0	818	55	0
2	B	666	0	646	29	0
2	E	680	0	668	34	0
2	H	683	0	681	50	0
2	K	678	0	679	43	0
3	C	1058	0	975	61	0
3	F	1115	0	1073	45	0
3	I	1164	0	1141	73	0
3	L	1143	0	1123	64	0
4	A	3	0	0	0	0
4	C	4	0	0	3	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	6	0	0	0	0
4	G	7	0	0	5	0
4	H	4	0	0	0	0
4	I	5	0	0	3	0
4	J	3	0	0	0	0
4	K	5	0	0	1	0
4	L	9	0	0	1	0
All	All	10354	0	10019	549	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 27.

All (549) 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)
3:I:77:CYS:SG	3:I:77:CYS:CB	2.05	1.45
3:C:68:SER:CB	3:C:69:ARG:HA	1.30	1.36
3:C:68:SER:CB	3:C:69:ARG:CA	2.20	1.20
1:D:98:GLU:CB	1:D:99:LEU:HA	1.74	1.16
3:I:69:ARG:HG2	3:I:69:ARG:HH11	1.07	1.12
3:C:68:SER:HB2	3:C:69:ARG:HA	1.16	1.11
4:G:2003:HOH:O	2:H:27:HIS:HD2	1.32	1.10
3:F:104:GLY:HA3	2:H:63:ARG:HD2	1.29	1.09
3:C:78:ASN:HB2	3:C:101:LEU:HD23	1.18	1.09
2:K:45:MET:O	2:K:46:LEU:HD12	1.54	1.07
3:C:68:SER:HB2	3:C:69:ARG:CA	1.80	1.05
3:C:167:ARG:HB2	4:C:2003:HOH:O	1.54	1.05
3:C:65:SER:HB2	3:C:89:LEU:O	1.57	1.04
3:F:75:ILE:HD13	3:F:146:PRO:HB2	1.39	1.04
3:C:68:SER:HB3	3:C:69:ARG:HA	1.07	1.03
1:G:36:LYS:O	1:G:37:ARG:HG2	1.59	1.02
3:C:78:ASN:HB2	3:C:101:LEU:CD2	1.89	1.01
3:L:177:ARG:HH11	3:L:177:ARG:HG3	1.24	1.01
3:I:175:TYR:O	3:I:185:TYR:HE1	1.44	0.99
3:I:90:ASN:HD22	3:I:94:GLU:HB2	1.30	0.94
3:F:195:GLN:HA	3:F:195:GLN:OE1	1.64	0.93
2:K:77:PHE:O	2:K:81:VAL:HG23	1.69	0.93
1:A:8:ARG:HG2	1:A:13:THR:HG23	1.52	0.92
3:C:78:ASN:CB	3:C:101:LEU:HD23	2.00	0.92
3:C:163:LEU:CD2	3:C:188:LEU:HD23	2.00	0.91
1:G:99:LEU:H	1:G:100:PRO:HD3	1.34	0.90
2:E:102:GLU:HA	2:E:105:MET:HE3	1.53	0.88
1:D:99:LEU:CB	1:D:100:PRO:HD3	2.03	0.88
3:I:144:GLY:HA3	3:I:145:GLN:HB2	1.56	0.88
1:G:68:ARG:HG2	1:G:68:ARG:HH11	1.36	0.87
3:C:163:LEU:HD23	3:C:188:LEU:HD23	1.52	0.87
3:F:75:ILE:CD1	3:F:146:PRO:HB2	2.05	0.86
3:L:62:VAL:O	3:L:63:LEU:HB2	1.74	0.86
1:G:68:ARG:HG2	1:G:68:ARG:NH1	1.89	0.85
3:L:176:ARG:NH1	3:L:185:TYR:HB3	1.91	0.85
1:G:94:SER:H	2:H:67:SER:HB2	1.41	0.85
3:I:69:ARG:HH11	3:I:69:ARG:CG	1.90	0.84
3:I:73:GLN:H	3:I:141:ASN:ND2	1.75	0.84
1:A:47:ASP:O	1:A:48:ASP:HB2	1.78	0.83
3:I:144:GLY:HA3	3:I:145:GLN:CB	2.09	0.83
3:I:69:ARG:HG2	3:I:69:ARG:NH1	1.77	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:HD13	2:B:103:LEU:HD23	1.61	0.82
1:G:66:THR:O	1:G:66:THR:HG22	1.78	0.82
3:C:68:SER:HB2	3:C:69:ARG:CB	2.10	0.81
3:L:76:PHE:HB3	3:L:101:LEU:HD11	1.62	0.81
3:L:177:ARG:HH11	3:L:177:ARG:CG	1.94	0.81
1:J:83:ASP:CG	1:J:84:THR:H	1.88	0.80
3:C:67:ASN:HA	3:C:91:PHE:HE1	1.45	0.80
3:C:73:GLN:H	3:C:141:ASN:ND2	1.79	0.80
4:G:2003:HOH:O	2:H:27:HIS:CD2	2.15	0.78
2:K:68:HIS:O	4:K:2003:HOH:O	2.02	0.78
3:C:68:SER:HB3	3:C:69:ARG:CA	2.00	0.78
1:J:104:LYS:HG3	1:J:105:PRO:HB3	1.66	0.78
3:I:73:GLN:H	3:I:141:ASN:HD21	1.30	0.77
3:I:88:TRP:HZ3	3:I:96:GLN:NE2	1.80	0.77
3:F:64:ARG:HD2	3:F:91:PHE:O	1.83	0.77
3:L:177:ARG:HG3	3:L:177:ARG:NH1	2.00	0.77
3:C:78:ASN:ND2	3:C:103:PRO:HA	2.00	0.77
3:L:76:PHE:O	3:L:106:GLY:HA2	1.85	0.77
1:D:98:GLU:CB	1:D:99:LEU:CA	2.61	0.76
3:I:141:ASN:OD1	3:I:145:GLN:O	2.03	0.76
1:D:79:PHE:H	1:D:86:GLU:HG2	1.51	0.76
3:I:175:TYR:O	3:I:185:TYR:CE1	2.35	0.75
2:H:34:GLU:N	2:H:34:GLU:OE1	2.19	0.75
1:D:99:LEU:CB	1:D:100:PRO:CD	2.64	0.74
3:F:67:ASN:HA	3:F:91:PHE:CE1	2.22	0.74
3:F:131:ASN:O	3:F:132:GLN:HB2	1.86	0.74
3:C:163:LEU:HD23	3:C:188:LEU:CD2	2.18	0.73
3:F:67:ASN:HA	3:F:91:PHE:HE1	1.53	0.73
3:F:165:VAL:O	3:F:169:LEU:HD12	1.88	0.73
3:F:204:GLU:C	3:F:204:GLU:OE1	2.32	0.73
3:F:69:ARG:HG3	3:F:69:ARG:HH11	1.55	0.72
3:C:160:GLU:HA	3:C:163:LEU:HD12	1.69	0.72
3:I:193:ASN:HB3	3:I:196:LYS:HB2	1.72	0.72
1:A:29:ARG:O	1:A:32:GLU:HB3	1.90	0.71
1:G:23:THR:OG1	1:G:26:GLU:HG3	1.90	0.71
1:J:83:ASP:O	1:J:84:THR:HG23	1.90	0.70
1:J:41:GLU:HA	1:J:80:ARG:HG2	1.72	0.70
2:E:34:GLU:CD	2:E:34:GLU:H	1.99	0.70
3:C:73:GLN:N	3:C:141:ASN:ND2	2.38	0.70
3:L:68:SER:HB2	3:L:70:GLU:HG2	1.73	0.70
1:J:9:ARG:HB2	1:J:77:LEU:HB3	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HG2	1:A:45:TYR:CE1	2.27	0.69
1:A:47:ASP:O	1:A:48:ASP:CB	2.40	0.69
1:G:66:THR:O	1:G:66:THR:CG2	2.39	0.69
1:J:41:GLU:CG	1:J:80:ARG:HG2	2.22	0.69
2:K:42:ILE:O	2:K:45:MET:HB2	1.92	0.69
1:D:51:LEU:HD22	1:D:60:CYS:SG	2.33	0.69
3:C:67:ASN:HA	3:C:91:PHE:CE1	2.28	0.69
3:C:130:VAL:HG11	3:C:136:PHE:HB2	1.75	0.69
3:L:64:ARG:HD2	3:L:91:PHE:O	1.94	0.67
3:C:163:LEU:HD22	3:C:188:LEU:HD23	1.76	0.67
3:L:70:GLU:HG3	3:L:113:ARG:HB2	1.75	0.67
3:L:131:ASN:O	3:L:132:GLN:HB2	1.93	0.67
2:K:103:LEU:HB3	3:L:162:CYS:SG	2.34	0.67
1:J:19:LYS:O	1:J:57:LEU:HD12	1.95	0.67
2:E:34:GLU:CD	2:E:34:GLU:N	2.53	0.67
3:L:120:ARG:NH1	3:L:197:ASP:OD2	2.27	0.67
2:E:104:LEU:HB2	3:F:162:CYS:HB3	1.77	0.67
1:G:70:GLN:O	4:G:2005:HOH:O	2.11	0.67
2:B:33:ARG:O	2:B:37:LEU:HG	1.95	0.66
1:A:43:ARG:HG3	1:A:50:LEU:HD11	1.77	0.66
3:L:102:PRO:HB2	3:L:103:PRO:HD2	1.75	0.66
2:H:76:TYR:C	2:H:76:TYR:CD1	2.73	0.66
2:E:71:SER:O	2:E:75:MET:HG3	1.96	0.66
1:G:32:GLU:OE1	1:G:39:PRO:HD3	1.95	0.66
3:F:73:GLN:OE1	3:F:110:HIS:CD2	2.49	0.66
1:G:27:LEU:O	1:G:31:VAL:HG23	1.96	0.65
3:L:181:VAL:O	3:L:182:ARG:C	2.38	0.65
3:I:131:ASN:O	3:I:132:GLN:HB2	1.96	0.65
1:D:19:LYS:O	1:D:22:SER:HB3	1.97	0.65
2:H:46:LEU:O	2:H:47:SER:O	2.13	0.65
3:I:88:TRP:HZ3	3:I:96:GLN:HE22	1.43	0.65
2:H:39:SER:HB3	2:H:42:ILE:HB	1.77	0.65
3:I:90:ASN:ND2	3:I:94:GLU:HB2	2.06	0.65
2:E:37:LEU:N	2:E:37:LEU:HD23	2.12	0.65
3:I:88:TRP:CZ3	3:I:96:GLN:NE2	2.63	0.65
3:L:141:ASN:O	3:L:142:VAL:C	2.41	0.64
2:K:19:VAL:HG22	2:K:31:VAL:O	1.98	0.64
2:H:73:VAL:HG12	2:H:77:PHE:CZ	2.32	0.64
1:D:28:LYS:HE2	1:D:53:ASP:OD1	1.98	0.64
3:I:90:ASN:HD22	3:I:94:GLU:CB	2.08	0.64
2:B:87:SER:O	2:B:88:THR:C	2.40	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:THR:O	2:H:89:GLU:C	2.41	0.64
1:G:52:ASP:HB2	1:G:55:LYS:CG	2.28	0.63
3:I:189:GLU:O	3:I:191:HIS:N	2.31	0.63
3:L:127:GLY:O	3:L:128:LEU:HD23	1.99	0.63
3:I:78:ASN:O	3:I:104:GLY:HA2	1.99	0.63
3:I:172:PRO:HD2	3:I:173:GLU:OE1	1.98	0.63
2:H:22:ILE:HA	2:H:27:HIS:O	1.99	0.63
1:G:28:LYS:HG2	1:G:42:GLN:NE2	2.14	0.63
2:K:62:PHE:HB3	2:K:65:ILE:HG13	1.80	0.63
3:C:130:VAL:CG1	3:C:136:PHE:HB2	2.29	0.62
3:L:90:ASN:HB2	3:L:94:GLU:O	1.99	0.62
1:G:56:THR:OG1	1:G:59:GLU:HG3	2.00	0.62
1:J:103:MET:O	1:J:104:LYS:HB2	1.98	0.62
2:K:44:ALA:C	2:K:46:LEU:H	2.07	0.62
3:C:137:VAL:HG12	3:C:137:VAL:O	2.00	0.62
1:J:1:MET:HE2	1:J:64:SER:CB	2.30	0.61
1:J:19:LYS:HB2	1:J:22:SER:HB3	1.81	0.61
2:K:20:LYS:HE2	2:K:30:ILE:HD11	1.81	0.61
3:F:67:ASN:CA	3:F:91:PHE:CE1	2.83	0.61
1:J:83:ASP:CG	1:J:84:THR:N	2.57	0.61
1:G:8:ARG:NH2	1:G:91:GLU:O	2.34	0.61
3:C:73:GLN:N	3:C:141:ASN:HD21	1.98	0.60
3:C:164:GLN:HA	4:C:2003:HOH:O	2.02	0.60
3:C:141:ASN:O	3:C:142:VAL:O	2.20	0.60
1:J:26:GLU:O	1:J:29:ARG:HB2	2.02	0.60
1:A:29:ARG:NH1	1:A:32:GLU:OE1	2.34	0.60
2:E:37:LEU:HD23	2:E:37:LEU:H	1.65	0.60
2:B:95:ILE:HD13	2:B:103:LEU:CD2	2.31	0.60
1:G:32:GLU:OE1	1:G:38:PRO:HA	2.01	0.59
1:D:28:LYS:NZ	1:D:43:ARG:HA	2.16	0.59
1:D:1:MET:HE1	2:E:82:ARG:HH22	1.68	0.59
1:G:97:PRO:O	1:G:98:GLU:HB2	2.03	0.59
2:H:73:VAL:CG1	2:H:77:PHE:CZ	2.86	0.59
1:J:1:MET:O	1:J:19:LYS:HA	2.02	0.59
1:J:28:LYS:HE2	1:J:53:ASP:OD1	2.02	0.59
3:L:140:LEU:O	3:L:141:ASN:O	2.21	0.58
1:D:42:GLN:HE21	1:D:77:LEU:HD13	1.69	0.58
2:B:102:GLU:HA	2:B:105:MET:HE3	1.84	0.58
3:I:69:ARG:HG3	4:I:2003:HOH:O	2.03	0.58
3:C:78:ASN:O	3:C:103:PRO:O	2.21	0.58
3:C:84:VAL:O	3:C:100:THR:HG22	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:144:GLY:CA	3:I:145:GLN:CB	2.82	0.58
1:J:41:GLU:HG2	1:J:80:ARG:CG	2.34	0.58
3:I:112:TYR:O	3:I:138:PRO:HB2	2.03	0.58
1:J:3:VAL:HG22	1:J:18:ALA:O	2.04	0.58
3:L:160:GLU:O	3:L:164:GLN:HG3	2.03	0.58
1:J:80:ARG:HA	1:J:85:PHE:HA	1.86	0.57
2:H:36:ALA:HB1	2:H:42:ILE:HG21	1.85	0.57
3:I:69:ARG:CG	4:I:2003:HOH:O	2.50	0.57
2:H:18:TYR:O	2:H:19:VAL:HG12	2.04	0.57
3:L:184:LEU:O	3:L:188:LEU:HB2	2.03	0.57
3:F:67:ASN:CA	3:F:91:PHE:HE1	2.17	0.57
1:G:72:PRO:HD2	2:H:75:MET:HE2	1.86	0.57
1:A:68:ARG:O	1:A:71:ALA:N	2.37	0.57
2:B:104:LEU:HB2	3:C:162:CYS:HB3	1.87	0.57
3:C:67:ASN:C	3:C:67:ASN:HD22	2.12	0.57
1:J:37:ARG:HH12	1:J:41:GLU:HG2	1.69	0.57
2:E:33:ARG:O	2:E:37:LEU:HD23	2.05	0.57
3:F:90:ASN:HB3	3:F:92:ASP:H	1.69	0.57
3:I:157:THR:OG1	3:I:160:GLU:HB2	2.04	0.57
3:I:164:GLN:O	3:I:168:SER:HB3	2.04	0.57
2:B:87:SER:O	2:B:89:GLU:N	2.37	0.56
1:D:29:ARG:O	1:D:32:GLU:HB3	2.04	0.56
3:I:90:ASN:HB3	3:I:92:ASP:H	1.70	0.56
1:J:41:GLU:CG	1:J:80:ARG:CG	2.83	0.56
2:K:19:VAL:O	2:K:30:ILE:HA	2.04	0.56
2:B:98:GLU:H	2:B:98:GLU:CD	2.14	0.56
3:F:163:LEU:HD22	3:F:188:LEU:HD23	1.86	0.56
1:G:79:PHE:O	1:G:85:PHE:CD1	2.59	0.56
1:J:37:ARG:NH1	1:J:41:GLU:HG2	2.21	0.56
3:C:142:VAL:O	3:C:143:ASP:C	2.48	0.56
1:D:44:LEU:HD23	1:D:77:LEU:HB2	1.86	0.56
3:C:78:ASN:HD21	3:C:103:PRO:HA	1.67	0.56
1:J:1:MET:HE2	1:J:64:SER:HB3	1.87	0.56
2:E:110:LEU:O	2:E:111:ASP:HB3	2.06	0.56
2:K:25:ASP:N	2:K:25:ASP:OD1	2.33	0.56
3:I:166:VAL:HG11	3:I:188:LEU:HD11	1.87	0.55
1:J:94:SER:O	2:K:68:HIS:HB3	2.07	0.55
1:A:22:SER:OG	1:A:57:LEU:HD12	2.06	0.55
3:C:105:THR:HG22	2:K:64:GLU:OE1	2.07	0.55
3:C:145:GLN:CB	3:C:146:PRO:HD3	2.36	0.55
3:F:120:ARG:NH1	3:F:197:ASP:OD2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:OG1	1:A:59:GLU:HB2	2.06	0.55
1:J:66:THR:HG22	1:J:66:THR:O	2.05	0.55
3:F:174:ASN:HD22	3:F:174:ASN:N	2.05	0.55
1:G:22:SER:HB2	1:G:26:GLU:OE1	2.07	0.55
1:A:32:GLU:O	1:A:36:LYS:HA	2.06	0.55
1:D:70:GLN:HG3	2:E:79:TYR:CD1	2.40	0.55
2:E:23:SER:HA	2:E:70:LEU:HD23	1.88	0.55
1:G:8:ARG:NH2	4:G:2001:HOH:O	2.38	0.55
1:J:4:PHE:CE2	1:J:69:PRO:HG3	2.41	0.55
2:K:35:HIS:HD2	2:K:78:THR:HG22	1.71	0.55
1:G:10:HIS:O	1:G:91:GLU:HB2	2.07	0.55
3:I:73:GLN:HB2	3:I:141:ASN:HD21	1.71	0.55
1:G:52:ASP:HB2	1:G:55:LYS:HG2	1.88	0.54
1:G:99:LEU:N	1:G:100:PRO:HD3	2.13	0.54
1:G:52:ASP:HB2	1:G:55:LYS:HG3	1.89	0.54
3:L:70:GLU:O	3:L:112:TYR:HA	2.07	0.54
1:A:65:GLN:O	1:A:68:ARG:HD2	2.06	0.54
2:B:37:LEU:O	2:B:38:THR:C	2.50	0.54
3:I:129:LEU:HG	3:I:154:PRO:HB3	1.87	0.54
1:J:41:GLU:HG3	1:J:80:ARG:HG2	1.87	0.54
2:H:104:LEU:HB2	3:I:162:CYS:HB3	1.90	0.54
2:B:76:TYR:CD1	2:B:76:TYR:C	2.85	0.54
1:J:51:LEU:HD22	1:J:60:CYS:SG	2.48	0.54
1:G:28:LYS:HD3	1:G:42:GLN:HB3	1.89	0.54
1:G:92:PRO:HA	4:G:2002:HOH:O	2.07	0.54
3:F:86:PRO:HB3	3:F:119:PHE:HE1	1.70	0.54
3:F:89:LEU:HD12	3:F:116:LEU:HD23	1.89	0.54
1:D:70:GLN:HG3	2:E:79:TYR:HD1	1.74	0.53
1:J:11:LYS:HG3	1:J:91:GLU:HG3	1.91	0.53
1:J:23:THR:HG1	1:J:26:GLU:HG3	1.73	0.53
1:G:3:VAL:HG22	1:G:67:ALA:HB3	1.90	0.53
2:K:72:LYS:O	2:K:73:VAL:C	2.48	0.53
1:G:7:ILE:HD13	1:G:31:VAL:HG22	1.91	0.53
2:B:42:ILE:HG12	2:B:62:PHE:HZ	1.73	0.53
1:A:15:PHE:HB2	2:B:31:VAL:HG22	1.90	0.53
1:G:72:PRO:HD3	2:H:75:MET:HG2	1.90	0.53
1:D:70:GLN:H	1:D:70:GLN:NE2	2.06	0.53
1:G:98:GLU:HB3	1:G:99:LEU:CB	2.38	0.53
2:B:89:GLU:HG3	3:C:79:ARG:HB3	1.90	0.52
3:I:160:GLU:O	3:I:164:GLN:HG3	2.09	0.52
3:F:118:LEU:C	3:F:118:LEU:HD12	2.33	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:LYS:O	2:H:84:THR:HB	2.09	0.52
3:L:140:LEU:C	3:L:141:ASN:O	2.52	0.52
3:I:66:VAL:HG23	3:I:114:GLY:O	2.09	0.52
3:L:129:LEU:HD11	3:L:154:PRO:HB3	1.92	0.52
3:F:84:VAL:HG21	3:F:151:ILE:HG21	1.91	0.52
3:F:86:PRO:HB3	3:F:119:PHE:CE1	2.44	0.52
2:E:27:HIS:ND1	2:E:67:SER:OG	2.43	0.52
2:E:39:SER:OG	2:E:110:LEU:O	2.26	0.52
3:F:68:SER:O	3:F:68:SER:OG	2.25	0.52
3:L:130:VAL:HG13	3:L:130:VAL:O	2.09	0.52
2:B:84:THR:O	2:B:85:ASN:HB2	2.09	0.52
2:B:42:ILE:O	2:B:43:LYS:C	2.51	0.51
3:F:78:ASN:HB2	3:F:101:LEU:HD13	1.91	0.51
1:G:68:ARG:HH11	1:G:68:ARG:CG	2.06	0.51
3:I:129:LEU:HD13	3:I:132:GLN:O	2.10	0.51
2:K:40:GLY:O	2:K:43:LYS:HB3	2.11	0.51
3:C:78:ASN:ND2	3:C:103:PRO:CA	2.73	0.51
3:I:74:VAL:HG12	3:I:109:ILE:HB	1.92	0.51
2:K:20:LYS:NZ	2:K:28:GLU:CD	2.69	0.51
2:H:76:TYR:CD2	3:I:158:LEU:HB2	2.46	0.51
3:L:78:ASN:OD1	3:L:78:ASN:C	2.52	0.51
3:L:112:TYR:HB2	3:L:115:HIS:CE1	2.46	0.51
3:L:192:PRO:HA	4:L:2009:HOH:O	2.09	0.51
3:C:181:VAL:O	3:C:184:LEU:HB2	2.11	0.51
2:E:35:HIS:HD2	2:E:78:THR:HG22	1.74	0.51
1:G:46:LYS:HD2	1:G:62:PHE:CZ	2.45	0.51
1:J:104:LYS:HG3	1:J:105:PRO:CB	2.38	0.51
2:E:33:ARG:O	2:E:37:LEU:HG	2.11	0.51
2:H:18:TYR:C	2:H:19:VAL:CG1	2.84	0.51
3:I:70:GLU:O	3:I:112:TYR:HA	2.11	0.51
3:C:65:SER:OG	3:C:115:HIS:HA	2.11	0.50
3:I:73:GLN:N	3:I:141:ASN:HD21	2.03	0.50
1:G:28:LYS:HE2	1:G:42:GLN:O	2.11	0.50
3:L:140:LEU:HD23	3:L:141:ASN:O	2.11	0.50
1:D:42:GLN:HE21	1:D:77:LEU:CD1	2.24	0.50
3:L:72:SER:OG	3:L:139:SER:O	2.29	0.50
1:G:94:SER:H	2:H:67:SER:CB	2.18	0.50
2:H:35:HIS:CE1	2:H:81:VAL:HG11	2.46	0.50
1:J:103:MET:O	1:J:104:LYS:CB	2.60	0.50
2:E:37:LEU:N	2:E:37:LEU:CD2	2.75	0.50
3:C:75:ILE:HG22	3:C:146:PRO:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:ASN:OD1	3:F:159:LYS:HE3	2.11	0.50
1:J:65:GLN:O	1:J:68:ARG:HD2	2.11	0.50
1:D:28:LYS:HZ1	1:D:43:ARG:HA	1.77	0.49
1:D:69:PRO:HD2	1:D:70:GLN:HE22	1.75	0.49
1:G:28:LYS:HA	1:G:42:GLN:HE22	1.77	0.49
3:I:130:VAL:O	3:I:130:VAL:HG13	2.11	0.49
1:J:15:PHE:HE1	2:K:29:PHE:HD1	1.59	0.49
1:D:70:GLN:H	1:D:70:GLN:CD	2.19	0.49
1:G:97:PRO:O	1:G:98:GLU:CB	2.60	0.49
3:L:84:VAL:HG12	3:L:85:LEU:N	2.28	0.49
2:E:33:ARG:O	2:E:37:LEU:CD2	2.60	0.49
3:L:112:TYR:O	3:L:113:ARG:C	2.54	0.49
2:K:45:MET:C	2:K:46:LEU:HD12	2.33	0.49
2:K:45:MET:O	2:K:46:LEU:CD1	2.44	0.49
1:G:68:ARG:HD3	1:G:71:ALA:HB3	1.95	0.49
1:J:47:ASP:O	1:J:48:ASP:HB2	2.12	0.49
3:C:112:TYR:O	3:C:113:ARG:C	2.56	0.48
1:J:100:PRO:O	1:J:102:VAL:HG22	2.12	0.48
3:C:102:PRO:HG2	3:C:105:THR:HG21	1.94	0.48
2:H:103:LEU:HG	3:I:158:LEU:HD11	1.93	0.48
1:J:1:MET:HE2	1:J:64:SER:OG	2.12	0.48
1:A:100:PRO:O	1:A:101:ASP:CB	2.61	0.48
1:G:16:THR:OG1	1:G:17:ASP:N	2.45	0.48
1:J:41:GLU:HG2	1:J:80:ARG:HG3	1.94	0.48
3:L:141:ASN:O	3:L:142:VAL:O	2.30	0.48
1:J:9:ARG:HG3	1:J:77:LEU:O	2.14	0.48
2:E:102:GLU:O	2:E:103:LEU:C	2.56	0.48
3:C:172:PRO:HA	3:C:175:TYR:CB	2.44	0.48
1:D:3:VAL:HG21	1:D:62:PHE:O	2.14	0.48
2:H:96:ALA:HA	2:H:97:PRO:HD2	1.71	0.48
3:C:120:ARG:C	3:C:128:LEU:HD12	2.39	0.48
2:H:104:LEU:O	2:H:107:ALA:HB3	2.14	0.48
1:A:45:TYR:HD2	1:A:48:ASP:O	1.97	0.48
1:A:68:ARG:O	1:A:71:ALA:C	2.57	0.48
2:B:79:TYR:CZ	2:B:93:PHE:HB2	2.49	0.48
1:J:70:GLN:O	1:J:70:GLN:HG2	2.11	0.48
1:G:99:LEU:H	1:G:100:PRO:CD	2.16	0.48
3:I:173:GLU:CD	3:I:173:GLU:H	2.19	0.48
3:L:141:ASN:C	3:L:142:VAL:O	2.57	0.48
3:L:102:PRO:CB	3:L:103:PRO:HD2	2.42	0.47
3:L:115:HIS:O	3:L:116:LEU:HD12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:THR:OG1	1:J:26:GLU:HG3	2.14	0.47
1:J:72:PRO:HD3	2:K:75:MET:HG2	1.96	0.47
3:L:176:ARG:HH12	3:L:185:TYR:HB3	1.70	0.47
1:A:51:LEU:HD22	1:A:60:CYS:SG	2.55	0.47
3:L:160:GLU:HA	3:L:163:LEU:HD12	1.96	0.47
1:D:26:GLU:O	1:D:29:ARG:HB2	2.14	0.47
3:C:78:ASN:CB	3:C:101:LEU:CD2	2.75	0.47
1:D:3:VAL:HG22	1:D:67:ALA:HB3	1.95	0.47
3:I:84:VAL:HG22	3:I:128:LEU:HD13	1.97	0.47
3:F:142:VAL:O	3:F:143:ASP:C	2.57	0.47
3:F:166:VAL:O	3:F:167:ARG:C	2.57	0.47
3:I:90:ASN:C	3:I:92:ASP:N	2.72	0.47
1:G:69:PRO:HB3	2:H:78:THR:HG22	1.97	0.47
2:H:34:GLU:O	2:H:37:LEU:HB2	2.15	0.47
2:H:61:ASN:O	2:H:63:ARG:NH1	2.47	0.47
2:H:95:ILE:HB	3:I:165:VAL:HG21	1.96	0.47
3:I:137:VAL:HA	3:I:138:PRO:HD2	1.75	0.47
3:I:172:PRO:CD	3:I:173:GLU:OE1	2.62	0.47
2:K:89:GLU:O	2:K:89:GLU:HG2	2.14	0.47
3:L:101:LEU:HD21	3:L:107:ARG:HG2	1.96	0.47
2:K:79:TYR:CE2	2:K:93:PHE:HB2	2.50	0.47
2:K:25:ASP:OD2	2:K:67:SER:HB3	2.15	0.47
2:E:69:VAL:O	2:E:73:VAL:HG23	2.15	0.46
2:H:72:LYS:O	2:H:73:VAL:C	2.58	0.46
3:F:164:GLN:O	3:F:168:SER:HB3	2.16	0.46
2:H:96:ALA:O	2:H:97:PRO:C	2.59	0.46
3:I:157:THR:OG1	3:I:160:GLU:N	2.40	0.46
1:A:31:VAL:O	1:A:32:GLU:C	2.58	0.46
1:J:44:LEU:HD21	1:J:77:LEU:HD13	1.96	0.46
2:E:89:GLU:HG3	3:F:79:ARG:O	2.14	0.46
3:F:179:ASP:O	3:F:180:ILE:HG23	2.16	0.46
1:G:36:LYS:C	1:G:37:ARG:HG2	2.34	0.46
3:L:70:GLU:CG	3:L:113:ARG:HB2	2.43	0.46
1:G:79:PHE:H	1:G:86:GLU:HG2	1.81	0.46
3:L:131:ASN:O	3:L:132:GLN:CB	2.60	0.46
3:C:130:VAL:O	3:C:131:ASN:C	2.59	0.46
1:G:63:THR:O	1:G:64:SER:C	2.58	0.46
1:G:100:PRO:HD2	1:G:103:MET:HG3	1.98	0.46
2:H:73:VAL:HG12	2:H:77:PHE:CE2	2.50	0.46
2:H:88:THR:O	2:H:89:GLU:O	2.33	0.46
1:J:5:LEU:HA	1:J:73:ALA:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:H	2:B:67:SER:HB2	1.80	0.46
2:B:38:THR:HG21	2:B:80:LYS:HD3	1.98	0.46
2:B:67:SER:C	2:B:69:VAL:H	2.24	0.46
3:C:154:PRO:HD2	3:C:156:TYR:CZ	2.50	0.46
1:D:56:THR:OG1	1:D:59:GLU:HB2	2.16	0.46
3:L:67:ASN:HB2	3:L:91:PHE:CE1	2.50	0.46
2:H:100:ALA:O	2:H:101:LEU:C	2.58	0.45
3:L:179:ASP:O	3:L:180:ILE:HG23	2.16	0.45
2:B:101:LEU:HD23	2:B:101:LEU:HA	1.64	0.45
1:G:98:GLU:CA	1:G:99:LEU:CB	2.94	0.45
1:D:4:PHE:CE2	1:D:69:PRO:HG3	2.51	0.45
3:L:172:PRO:HA	3:L:175:TYR:CE1	2.51	0.45
3:L:176:ARG:HD2	3:L:176:ARG:HA	1.64	0.45
3:F:193:ASN:HB3	3:F:196:LYS:HB2	1.98	0.45
1:G:98:GLU:HA	1:G:99:LEU:CB	2.46	0.45
3:C:192:PRO:HB3	4:C:2002:HOH:O	2.16	0.45
1:G:32:GLU:OE1	1:G:39:PRO:CD	2.63	0.45
2:K:82:ARG:O	2:K:82:ARG:HG3	2.16	0.45
3:L:176:ARG:CZ	3:L:189:GLU:OE2	2.65	0.45
1:A:41:GLU:HG3	1:A:81:ALA:C	2.42	0.45
3:C:74:VAL:HG11	3:C:136:PHE:HE2	1.82	0.45
1:J:79:PHE:O	1:J:86:GLU:HG2	2.16	0.45
1:A:101:ASP:O	1:A:102:VAL:HG13	2.17	0.45
3:C:193:ASN:OD1	3:C:195:GLN:CB	2.65	0.45
3:C:197:ASP:O	3:C:201:LEU:N	2.28	0.45
1:D:96:PRO:HA	1:D:97:PRO:HD2	1.68	0.45
3:F:69:ARG:HG3	3:F:69:ARG:NH1	2.23	0.45
2:K:34:GLU:OE1	2:K:34:GLU:N	2.37	0.45
2:H:34:GLU:HA	2:H:37:LEU:HG	1.99	0.45
2:K:76:TYR:OH	2:K:80:LYS:HG3	2.16	0.45
1:A:5:LEU:HD13	1:A:27:LEU:HD11	1.99	0.45
2:H:30:ILE:C	2:H:31:VAL:HG23	2.42	0.45
3:C:102:PRO:CB	3:C:103:PRO:HD2	2.46	0.44
2:E:69:VAL:HG21	2:E:102:GLU:HB3	1.99	0.44
2:K:44:ALA:C	2:K:46:LEU:N	2.75	0.44
1:D:47:ASP:O	1:D:48:ASP:CB	2.63	0.44
1:G:28:LYS:NZ	1:G:53:ASP:OD1	2.51	0.44
1:G:81:ALA:O	1:G:83:ASP:N	2.50	0.44
3:I:99:PRO:HB2	3:I:107:ARG:HH12	1.81	0.44
3:I:198:LEU:O	3:I:202:THR:OG1	2.26	0.44
3:L:174:ASN:N	3:L:174:ASN:HD22	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PRO:HB2	1:D:41:GLU:CG	2.47	0.44
3:I:96:GLN:HA	3:I:97:PRO:HD2	1.80	0.44
1:J:11:LYS:CG	1:J:91:GLU:HG3	2.46	0.44
2:E:41:THR:O	2:E:45:MET:HG3	2.17	0.44
3:L:96:GLN:HA	3:L:97:PRO:HD3	1.87	0.44
1:D:24:VAL:HB	1:D:53:ASP:HA	1.99	0.44
1:G:46:LYS:HB2	1:G:51:LEU:HD11	2.00	0.44
2:H:76:TYR:CE1	2:H:80:LYS:HB2	2.53	0.44
3:C:78:ASN:OD1	3:C:80:SER:HB3	2.18	0.44
1:G:102:VAL:O	3:I:170:VAL:HB	2.18	0.44
2:B:69:VAL:O	2:B:73:VAL:HG23	2.17	0.44
3:L:90:ASN:C	3:L:92:ASP:N	2.74	0.44
3:I:117:TRP:HB2	3:I:136:PHE:HB3	2.00	0.44
1:J:37:ARG:NH1	1:J:41:GLU:CG	2.80	0.44
1:A:22:SER:OG	1:A:57:LEU:CD1	2.66	0.44
2:K:79:TYR:CZ	2:K:93:PHE:HB2	2.53	0.44
3:L:82:ARG:HD2	3:L:121:ASP:OD2	2.17	0.44
1:A:7:ILE:HB	1:A:14:ILE:HB	2.00	0.43
3:L:115:HIS:C	3:L:116:LEU:HD12	2.43	0.43
3:L:142:VAL:C	3:L:144:GLY:N	2.69	0.43
3:C:86:PRO:HA	3:C:119:PHE:CD2	2.52	0.43
3:C:115:HIS:O	3:C:138:PRO:HD2	2.17	0.43
1:D:32:GLU:O	1:D:36:LYS:HA	2.18	0.43
1:D:66:THR:O	1:D:66:THR:HG22	2.18	0.43
1:G:6:MET:CE	1:G:74:THR:OG1	2.67	0.43
3:L:129:LEU:CD1	3:L:154:PRO:HA	2.48	0.43
2:E:42:ILE:HG12	2:E:62:PHE:HZ	1.83	0.43
2:B:20:LYS:HD3	2:B:28:GLU:HB3	2.01	0.43
3:F:143:ASP:O	3:F:145:GLN:N	2.44	0.43
1:J:44:LEU:CD2	1:J:77:LEU:HD13	2.48	0.43
2:K:103:LEU:HD22	3:L:158:LEU:HD11	2.00	0.43
1:D:69:PRO:HD2	1:D:70:GLN:NE2	2.34	0.43
2:H:18:TYR:O	2:H:19:VAL:CG1	2.66	0.43
2:H:61:ASN:HB3	2:H:63:ARG:HH22	1.83	0.43
2:H:101:LEU:HD21	3:I:178:LEU:HD22	2.00	0.43
3:I:142:VAL:O	3:I:143:ASP:C	2.62	0.43
2:K:100:ALA:HB1	3:L:166:VAL:HG23	2.00	0.43
3:F:170:VAL:HG22	3:F:175:TYR:CD1	2.53	0.43
1:G:81:ALA:C	1:G:83:ASP:H	2.27	0.43
1:G:3:VAL:HG22	1:G:67:ALA:CB	2.48	0.43
1:G:37:ARG:HA	1:G:38:PRO:HD2	1.70	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:112:TYR:HB2	3:I:115:HIS:CE1	2.53	0.43
2:E:99:ILE:O	2:E:100:ALA:C	2.61	0.43
2:K:44:ALA:O	2:K:46:LEU:N	2.50	0.43
3:L:165:VAL:O	3:L:169:LEU:HD12	2.19	0.43
2:B:65:ILE:HG23	2:B:69:VAL:CG1	2.48	0.43
1:J:52:ASP:CB	1:J:55:LYS:HG2	2.49	0.43
2:K:84:THR:HG22	3:L:155:VAL:HB	2.00	0.43
3:I:114:GLY:HA2	3:I:137:VAL:HG12	2.00	0.43
1:J:15:PHE:HE1	2:K:29:PHE:CD1	2.37	0.43
3:F:118:LEU:HD12	3:F:119:PHE:N	2.34	0.42
3:I:172:PRO:HA	3:I:175:TYR:CE1	2.53	0.42
3:F:96:GLN:HA	3:F:97:PRO:HD2	1.64	0.42
1:J:91:GLU:HA	1:J:92:PRO:HD3	1.84	0.42
2:K:83:TYR:HB3	2:K:90:ILE:HG12	2.01	0.42
1:A:7:ILE:HD11	1:A:27:LEU:HD22	2.02	0.42
2:E:63:ARG:N	2:E:63:ARG:CD	2.82	0.42
1:A:70:GLN:HG2	1:A:71:ALA:N	2.28	0.42
2:B:95:ILE:CD1	2:B:103:LEU:HD23	2.40	0.42
1:G:15:PHE:CE2	2:H:74:CYS:HB2	2.55	0.42
1:G:80:ARG:O	1:G:85:PHE:CE1	2.72	0.42
1:G:93:PHE:C	1:G:94:SER:O	2.62	0.42
2:K:20:LYS:HZ1	2:K:28:GLU:CD	2.23	0.42
2:H:18:TYR:CE1	2:H:32:LYS:HG3	2.54	0.42
3:I:113:ARG:C	3:I:115:HIS:H	2.27	0.42
3:C:72:SER:N	3:C:111:SER:O	2.53	0.42
3:I:170:VAL:O	3:I:175:TYR:HE1	2.02	0.42
3:L:84:VAL:CG1	3:L:85:LEU:N	2.82	0.42
3:F:162:CYS:O	3:F:163:LEU:C	2.62	0.42
2:K:101:LEU:HD23	2:K:101:LEU:HA	1.89	0.42
3:L:70:GLU:HB2	3:L:113:ARG:HB2	2.00	0.42
1:A:58:GLY:HA2	1:A:62:PHE:O	2.20	0.42
3:C:183:SER:OG	3:C:184:LEU:N	2.51	0.42
2:E:107:ALA:HB2	3:F:158:LEU:HG	2.02	0.42
1:G:44:LEU:HA	1:G:76:GLY:O	2.20	0.42
1:G:56:THR:HG1	1:G:59:GLU:HG3	1.85	0.42
1:G:70:GLN:HG2	2:H:79:TYR:CD1	2.55	0.42
2:H:90:ILE:HA	2:H:91:PRO:HD3	1.85	0.42
3:L:75:ILE:HD13	3:L:108:ARG:HG3	2.02	0.42
2:B:31:VAL:CG1	2:B:32:LYS:N	2.82	0.41
2:E:41:THR:O	2:E:42:ILE:C	2.62	0.41
2:H:20:LYS:HE2	2:H:30:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:176:ARG:HA	3:I:176:ARG:HD3	1.89	0.41
3:L:85:LEU:HB2	3:L:122:ALA:HB2	2.02	0.41
2:B:20:LYS:HE3	2:B:20:LYS:HB2	1.88	0.41
2:E:19:VAL:HG13	2:E:33:ARG:HG3	2.00	0.41
3:F:75:ILE:CD1	3:F:146:PRO:CB	2.89	0.41
2:H:76:TYR:O	2:H:79:TYR:HB3	2.20	0.41
3:I:87:VAL:HB	3:I:118:LEU:HD12	2.02	0.41
3:I:180:ILE:O	3:I:185:TYR:CE2	2.73	0.41
1:J:32:GLU:C	1:J:34:ILE:N	2.76	0.41
2:K:90:ILE:HA	2:K:91:PRO:HD3	1.89	0.41
1:A:98:GLU:OE1	1:A:98:GLU:HA	2.20	0.41
3:C:121:ASP:O	3:C:125:HIS:N	2.49	0.41
1:G:91:GLU:HA	1:G:92:PRO:HD2	1.83	0.41
1:D:63:THR:C	1:D:65:GLN:N	2.79	0.41
3:F:68:SER:O	3:F:70:GLU:N	2.52	0.41
3:C:74:VAL:HG12	3:C:75:ILE:N	2.36	0.41
2:E:29:PHE:CD2	2:E:70:LEU:HG	2.56	0.41
3:I:84:VAL:HG22	3:I:128:LEU:CD1	2.51	0.41
1:A:3:VAL:O	1:A:17:ASP:HA	2.20	0.41
1:D:34:ILE:C	1:D:36:LYS:H	2.29	0.41
2:E:34:GLU:O	2:E:35:HIS:C	2.64	0.41
2:E:93:PHE:HA	2:E:94:PRO:HD3	1.78	0.41
2:H:25:ASP:OD1	2:H:67:SER:OG	2.36	0.41
3:I:134:GLU:HG2	3:I:201:LEU:HD11	2.03	0.41
1:J:32:GLU:O	1:J:33:GLY:C	2.61	0.41
1:J:38:PRO:HD2	1:J:41:GLU:HB2	2.02	0.41
1:D:63:THR:O	1:D:65:GLN:N	2.54	0.41
2:H:107:ALA:HB2	3:I:158:LEU:HG	2.03	0.41
1:A:99:LEU:HA	1:A:100:PRO:HD3	1.72	0.41
2:B:67:SER:C	2:B:69:VAL:N	2.79	0.41
2:B:101:LEU:O	2:B:102:GLU:C	2.63	0.41
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.64	0.41
1:G:35:LEU:HD23	1:G:35:LEU:HA	1.74	0.41
1:G:104:LYS:HA	1:G:105:PRO:HD3	1.92	0.41
1:J:7:ILE:HB	1:J:14:ILE:HB	2.01	0.41
1:J:9:ARG:O	1:J:10:HIS:HB2	2.20	0.41
1:J:104:LYS:CG	1:J:105:PRO:HB3	2.44	0.41
3:L:74:VAL:HA	3:L:147:ILE:O	2.21	0.41
3:I:119:PHE:CD1	3:I:119:PHE:N	2.88	0.41
2:K:36:ALA:C	2:K:38:THR:H	2.27	0.41
2:H:18:TYR:C	2:H:19:VAL:HG13	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:69:ARG:HG2	4:I:2003:HOH:O	2.16	0.40
2:K:21:LEU:HD22	2:K:62:PHE:HE2	1.86	0.40
2:K:36:ALA:C	2:K:38:THR:N	2.80	0.40
3:L:68:SER:CB	3:L:70:GLU:HG2	2.47	0.40
3:I:111:SER:C	3:I:112:TYR:CD2	2.99	0.40
1:A:70:GLN:HB3	2:B:79:TYR:HD2	1.86	0.40
2:H:62:PHE:C	2:H:64:GLU:N	2.79	0.40
3:I:195:GLN:O	3:I:199:GLU:N	2.51	0.40
2:K:41:THR:HG22	2:K:42:ILE:N	2.36	0.40
2:K:63:ARG:HB2	2:K:63:ARG:HH11	1.86	0.40
3:F:204:GLU:OE1	3:F:204:GLU:CA	2.69	0.40
3:L:70:GLU:HG3	3:L:113:ARG:HD3	2.04	0.40
3:F:74:VAL:C	3:F:75:ILE:HD12	2.46	0.40
3:F:167:ARG:NH2	3:F:187:ASP:O	2.52	0.40
3:I:119:PHE:CE1	3:I:130:VAL:HG21	2.57	0.40
3:I:128:LEU:HD23	3:I:128:LEU:HA	1.92	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	97/118 (82%)	84 (87%)	9 (9%)	4 (4%)	2	8
1	D	94/118 (80%)	77 (82%)	10 (11%)	7 (7%)	1	2
1	G	103/118 (87%)	81 (79%)	17 (16%)	5 (5%)	1	6
1	J	103/118 (87%)	88 (85%)	11 (11%)	4 (4%)	2	8
2	B	82/97 (84%)	64 (78%)	12 (15%)	6 (7%)	1	2
2	E	83/97 (86%)	74 (89%)	5 (6%)	4 (5%)	2	6
2	H	82/97 (84%)	65 (79%)	15 (18%)	2 (2%)	4	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	81/97 (84%)	68 (84%)	7 (9%)	6 (7%)	1	2
3	C	140/163 (86%)	108 (77%)	23 (16%)	9 (6%)	1	3
3	F	140/163 (86%)	113 (81%)	18 (13%)	9 (6%)	1	3
3	I	143/163 (88%)	116 (81%)	21 (15%)	6 (4%)	2	7
3	L	141/163 (86%)	123 (87%)	12 (8%)	6 (4%)	2	7
All	All	1289/1512 (85%)	1061 (82%)	160 (12%)	68 (5%)	1	5

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ASP
3	C	90	ASN
3	C	142	VAL
1	D	10	HIS
1	D	47	ASP
1	D	94	SER
1	D	97	PRO
1	D	99	LEU
1	D	100	PRO
3	F	144	GLY
3	F	145	GLN
1	G	82	ASP
1	G	99	LEU
3	I	145	GLN
3	I	190	ASP
3	I	205	ARG
1	J	102	VAL
2	K	41	THR
2	K	45	MET
3	L	63	LEU
3	L	90	ASN
3	L	141	ASN
3	L	182	ARG
3	L	190	ASP
1	A	20	GLU
1	A	48	ASP
1	A	80	ARG
2	B	85	ASN
2	B	88	THR
2	B	97	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	145	GLN
3	F	69	ARG
3	F	90	ASN
1	G	84	THR
2	H	89	GLU
2	K	42	ILE
3	L	142	VAL
2	B	89	GLU
3	C	68	SER
3	C	143	ASP
1	D	64	SER
2	E	37	LEU
2	E	87	SER
3	I	90	ASN
3	I	204	GLU
1	J	104	LYS
2	B	44	ALA
2	E	47	SER
3	F	132	GLN
3	F	179	ASP
1	G	94	SER
3	I	67	ASN
1	J	101	ASP
2	B	43	LYS
3	C	177	ARG
2	E	85	ASN
3	F	167	ARG
3	F	173	GLU
1	G	38	PRO
1	J	84	THR
2	K	89	GLU
3	C	83	VAL
2	K	98	GLU
2	K	97	PRO
2	H	97	PRO
3	C	103	PRO
3	C	191	HIS
3	F	103	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	82/103 (80%)	76 (93%)	6 (7%)	13	38
1	D	73/103 (71%)	59 (81%)	14 (19%)	1	5
1	G	87/103 (84%)	77 (88%)	10 (12%)	5	18
1	J	91/103 (88%)	84 (92%)	7 (8%)	12	36
2	B	72/86 (84%)	62 (86%)	10 (14%)	3	12
2	E	74/86 (86%)	61 (82%)	13 (18%)	2	7
2	H	76/86 (88%)	65 (86%)	11 (14%)	3	11
2	K	76/86 (88%)	69 (91%)	7 (9%)	8	27
3	C	107/149 (72%)	87 (81%)	20 (19%)	1	5
3	F	122/149 (82%)	101 (83%)	21 (17%)	2	7
3	I	129/149 (87%)	108 (84%)	21 (16%)	2	8
3	L	126/149 (85%)	112 (89%)	14 (11%)	6	20
All	All	1115/1352 (82%)	961 (86%)	154 (14%)	3	12

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	32	GLU
1	A	36	LYS
1	A	40	ASP
1	A	45	TYR
1	A	98	GLU
2	B	22	ILE
2	B	28	GLU
2	B	31	VAL
2	B	61	ASN
2	B	72	LYS
2	B	87	SER
2	B	95	ILE
2	B	97	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	98	GLU
2	B	99	ILE
3	C	65	SER
3	C	68	SER
3	C	75	ILE
3	C	77	CYS
3	C	80	SER
3	C	89	LEU
3	C	96	GLN
3	C	101	LEU
3	C	105	THR
3	C	116	LEU
3	C	137	VAL
3	C	141	ASN
3	C	148	PHE
3	C	166	VAL
3	C	180	ILE
3	C	184	LEU
3	C	186	GLU
3	C	194	VAL
3	C	198	LEU
3	C	202	THR
1	D	3	VAL
1	D	7	ILE
1	D	16	THR
1	D	22	SER
1	D	26	GLU
1	D	28	LYS
1	D	30	ILE
1	D	38	PRO
1	D	50	LEU
1	D	59	GLU
1	D	70	GLN
1	D	77	LEU
1	D	88	LEU
1	D	95	SER
2	E	17	MET
2	E	21	LEU
2	E	31	VAL
2	E	32	LYS
2	E	33	ARG
2	E	34	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	37	LEU
2	E	38	THR
2	E	70	LEU
2	E	78	THR
2	E	84	THR
2	E	88	THR
2	E	98	GLU
3	F	69	ARG
3	F	77	CYS
3	F	90	ASN
3	F	111	SER
3	F	116	LEU
3	F	120	ARG
3	F	138	PRO
3	F	139	SER
3	F	148	PHE
3	F	169	LEU
3	F	170	VAL
3	F	171	LYS
3	F	173	GLU
3	F	177	ARG
3	F	180	ILE
3	F	186	GLU
3	F	195	GLN
3	F	196	LYS
3	F	198	LEU
3	F	202	THR
3	F	204	GLU
1	G	1	MET
1	G	3	VAL
1	G	6	MET
1	G	19	LYS
1	G	49	GLN
1	G	68	ARG
1	G	70	GLN
1	G	74	THR
1	G	94	SER
1	G	102	VAL
2	H	19	VAL
2	H	30	ILE
2	H	45	MET
2	H	46	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	60	VAL
2	H	63	ARG
2	H	70	LEU
2	H	80	LYS
2	H	84	THR
2	H	99	ILE
2	H	101	LEU
3	I	62	VAL
3	I	63	LEU
3	I	66	VAL
3	I	69	ARG
3	I	70	GLU
3	I	72	SER
3	I	74	VAL
3	I	77	CYS
3	I	79	ARG
3	I	80	SER
3	I	111	SER
3	I	116	LEU
3	I	137	VAL
3	I	139	SER
3	I	170	VAL
3	I	176	ARG
3	I	177	ARG
3	I	181	VAL
3	I	183	SER
3	I	194	VAL
3	I	196	LYS
1	J	12	THR
1	J	22	SER
1	J	41	GLU
1	J	53	ASP
1	J	64	SER
1	J	80	ARG
1	J	84	THR
2	K	20	LYS
2	K	60	VAL
2	K	63	ARG
2	K	67	SER
2	K	78	THR
2	K	80	LYS
2	K	99	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	63	LEU
3	L	72	SER
3	L	77	CYS
3	L	116	LEU
3	L	120	ARG
3	L	145	GLN
3	L	150	ASN
3	L	173	GLU
3	L	176	ARG
3	L	177	ARG
3	L	181	VAL
3	L	188	LEU
3	L	196	LYS
3	L	197	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	67	ASN
3	C	141	ASN
1	D	10	HIS
1	D	42	GLN
1	D	70	GLN
2	E	35	HIS
3	F	73	GLN
3	F	90	ASN
3	F	110	HIS
3	F	174	ASN
3	F	191	HIS
1	G	42	GLN
2	H	27	HIS
2	H	61	ASN
3	I	73	GLN
3	I	90	ASN
3	I	96	GLN
3	I	141	ASN
3	I	150	ASN
3	I	191	HIS
3	I	193	ASN
3	I	195	GLN
1	J	49	GLN
3	L	96	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	174	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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	101/118 (85%)	-0.32	5 (4%) 34 26	18, 30, 50, 64	0
1	D	98/118 (83%)	-0.02	3 (3%) 51 41	26, 42, 56, 63	0
1	G	105/118 (88%)	-0.04	2 (1%) 66 57	24, 45, 61, 76	0
1	J	105/118 (88%)	-0.43	0 100 100	17, 31, 51, 68	0
2	B	86/97 (88%)	-0.51	0 100 100	19, 30, 46, 51	0
2	E	87/97 (89%)	-0.30	0 100 100	21, 36, 49, 53	0
2	H	86/97 (88%)	-0.11	0 100 100	23, 38, 58, 61	0
2	K	85/97 (87%)	-0.29	1 (1%) 76 68	18, 31, 51, 56	0
3	C	142/163 (87%)	-0.02	2 (1%) 73 64	17, 41, 63, 65	0
3	F	142/163 (87%)	-0.20	0 100 100	20, 37, 59, 69	0
3	I	145/163 (88%)	-0.22	0 100 100	18, 34, 56, 61	0
3	L	143/163 (87%)	-0.38	2 (1%) 73 64	14, 28, 50, 56	0
All	All	1325/1512 (87%)	-0.23	15 (1%) 78 70	14, 35, 58, 76	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	101	ASP	4.8
1	G	82	ASP	3.3
1	D	84	THR	3.1
1	A	101	ASP	2.9
3	C	204	GLU	2.8
1	A	99	LEU	2.7
2	K	58	ASN	2.5
1	A	102	VAL	2.4
3	C	142	VAL	2.4
1	G	105	PRO	2.4
3	L	141	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	204	GLU	2.3
1	A	103	MET	2.2
1	D	100	PRO	2.1
1	A	80	ARG	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 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.