



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:47 PM UTC

PDB ID : 5CFK / pdb_00005cfk
Title : Crystal structure of Proliferating Cell Nuclear Antigen from Leishmania donovani at 3.2 Å resolution
Authors : Shukla, P.K.; Yadav, S.P.; Sharma, P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2015-07-08
Resolution : 3.20 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

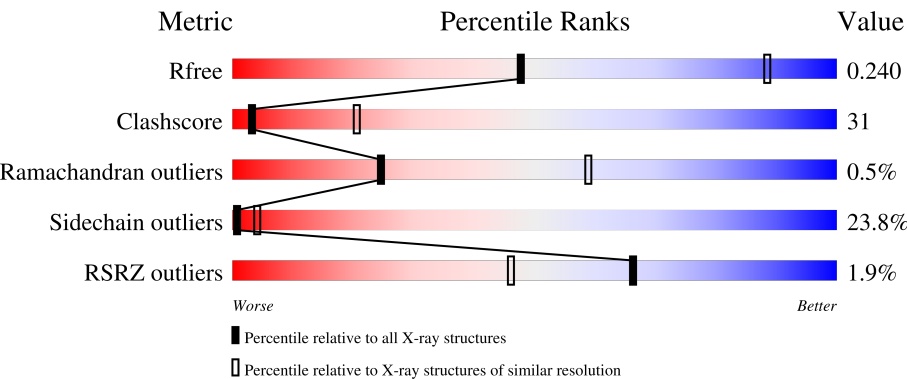
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	259	2% 46%42%9% .
1	B	259	2% 45%44%8% ..
1	C	259	% 42%39%16% ..
1	D	259	2% 39%47%11% .
1	E	259	2% 44%39%14% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	259	3% 42% 37% 17% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11739 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 Proliferating cell nuclear antigen,Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	B	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	C	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	D	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	E	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	F	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			

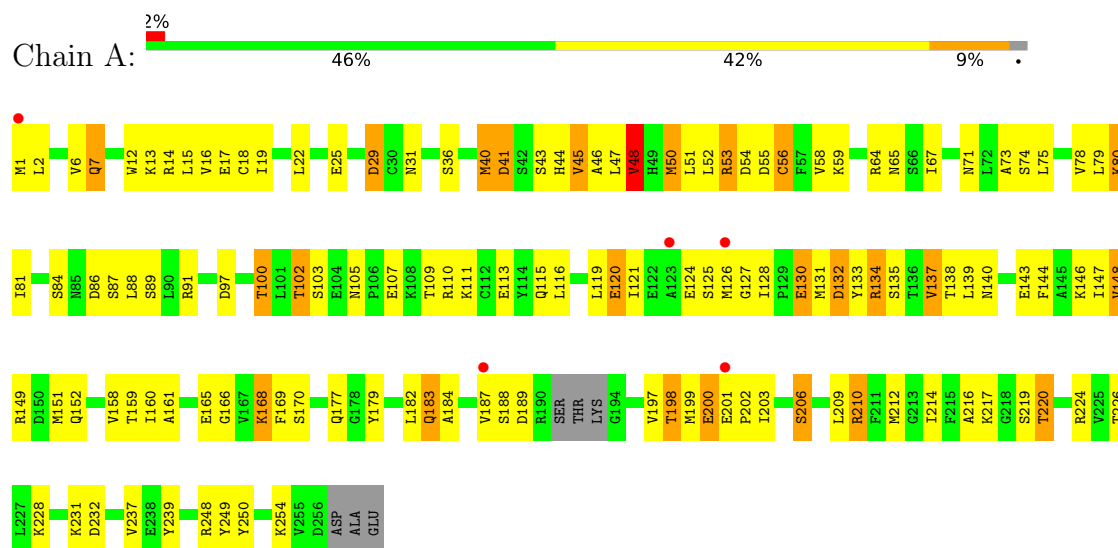
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		
2	F	3	Total	O	0	0
			3	3		

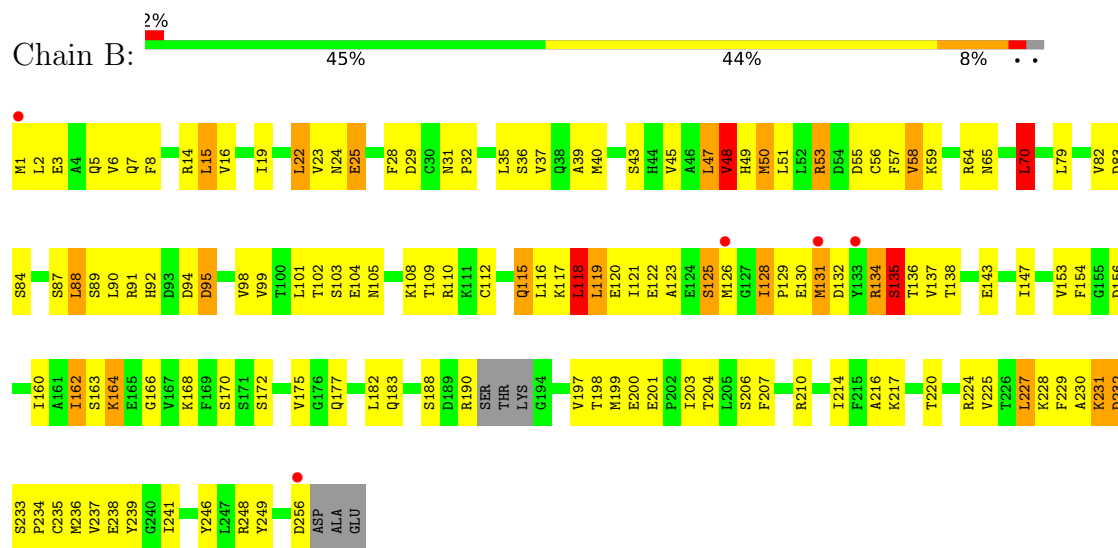
3 Residue-property plots [i](#)

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: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

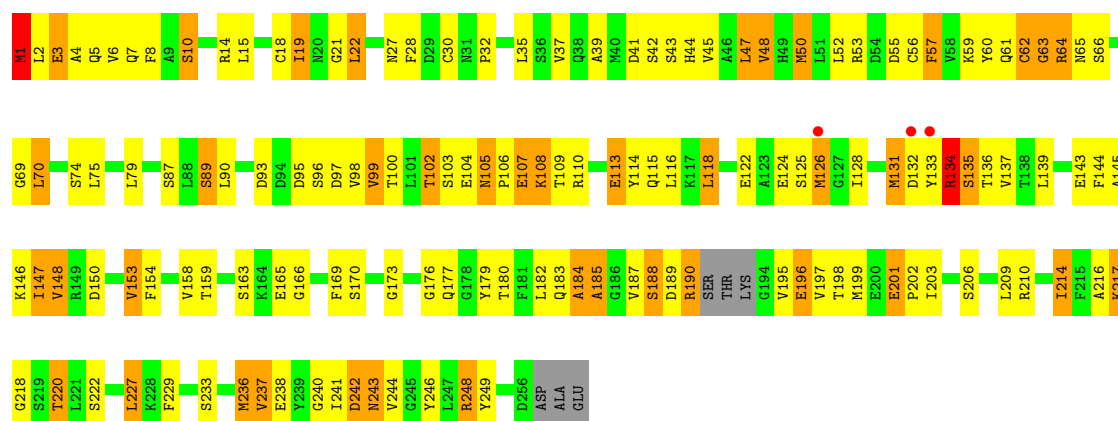


- Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

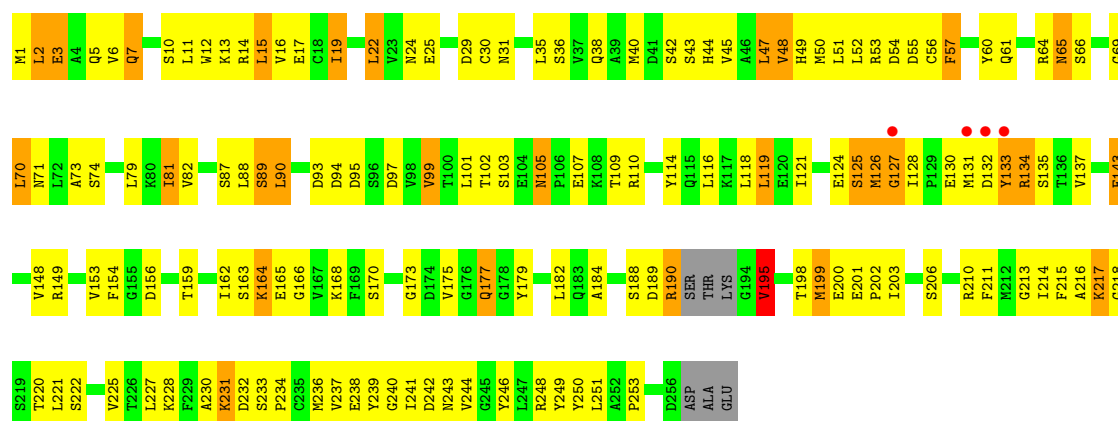


- Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

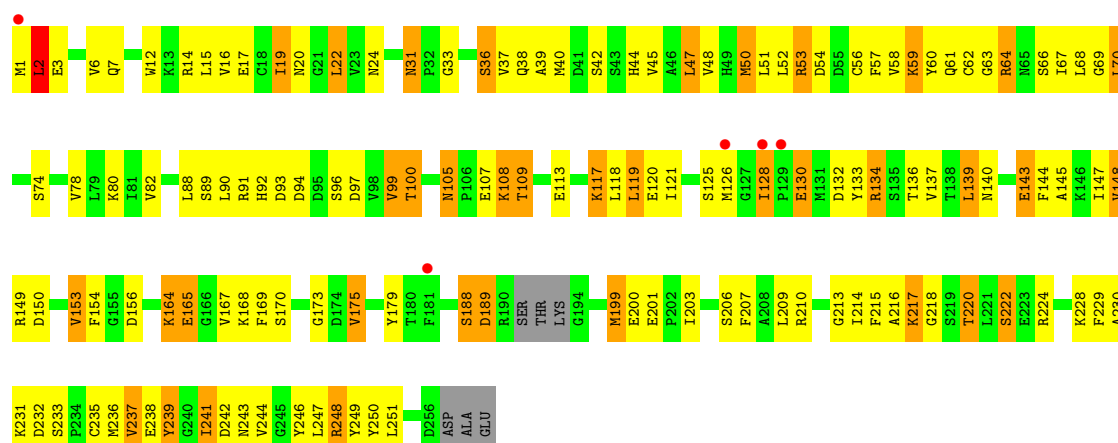
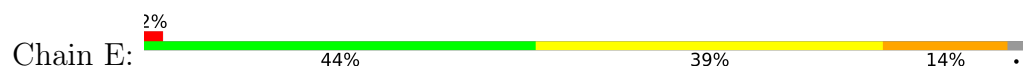




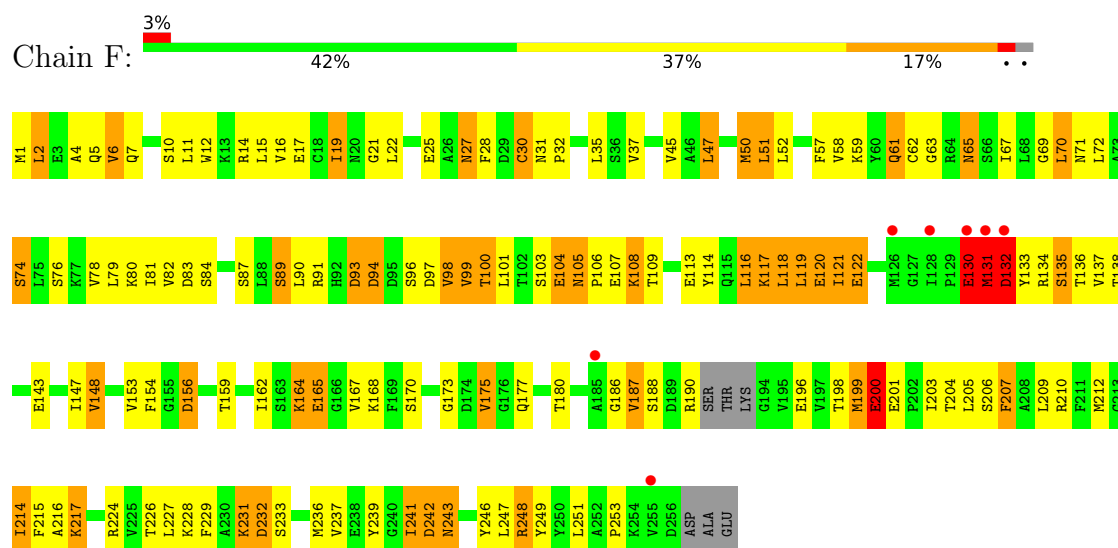
- Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.44Å 150.21Å 169.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.20) 99.6 (50.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.191 , 0.238 0.192 , 0.240	Depositor DCC
R_{free} test set	2854 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11739	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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	1.14	5/1983 (0.3%)	1.32	13/2675 (0.5%)
1	B	1.00	1/1983 (0.1%)	1.27	13/2675 (0.5%)
1	C	0.93	0/1983	1.31	16/2675 (0.6%)
1	D	0.96	2/1983 (0.1%)	1.25	9/2675 (0.3%)
1	E	0.92	1/1983 (0.1%)	1.26	13/2675 (0.5%)
1	F	1.10	14/1983 (0.7%)	1.25	10/2675 (0.4%)
All	All	1.01	23/11898 (0.2%)	1.28	74/16050 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	130	GLU	CD-OE1	10.01	1.44	1.25
1	D	190	ARG	C-O	9.53	1.42	1.23
1	F	188	SER	CB-OG	8.80	1.59	1.42
1	F	130	GLU	C-O	7.71	1.34	1.23
1	F	132	ASP	CG-OD1	7.62	1.39	1.25
1	F	131	MET	CG-SD	7.51	1.99	1.80
1	A	120	GLU	CD-OE2	7.35	1.39	1.25
1	F	131	MET	SD-CE	7.26	1.97	1.79
1	F	132	ASP	CB-CG	6.41	1.68	1.52
1	F	132	ASP	CG-OD2	6.33	1.37	1.25
1	F	132	ASP	C-O	6.30	1.31	1.23
1	A	132	ASP	C-O	6.18	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ASP	CG-OD1	6.15	1.37	1.25
1	A	120	GLU	CD-OE1	6.14	1.37	1.25
1	F	130	GLU	CA-CB	6.11	1.63	1.53
1	F	130	GLU	CG-CD	5.63	1.66	1.52
1	F	130	GLU	CD-OE2	5.55	1.35	1.25
1	B	117	LYS	CE-NZ	5.46	1.65	1.49
1	A	132	ASP	CG-OD2	5.37	1.35	1.25
1	F	106	PRO	N-CD	5.26	1.55	1.47
1	F	105	ASN	C-N	5.19	1.41	1.34
1	D	66	SER	N-CA	5.03	1.52	1.46
1	E	44	HIS	CG-CD2	5.02	1.41	1.35

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	185	ALA	N-CA-C	14.17	131.62	110.64
1	C	185	ALA	CB-CA-C	-13.95	92.64	109.80
1	B	48	VAL	CB-CA-C	-12.03	94.02	110.98
1	A	184	ALA	N-CA-C	9.15	124.02	112.03
1	D	188	SER	N-CA-C	9.00	123.89	111.74
1	C	105	ASN	CA-C-N	-8.99	110.72	119.89
1	C	105	ASN	C-N-CA	-8.99	110.72	119.89
1	B	70	LEU	N-CA-C	7.91	120.16	108.60
1	A	198	THR	N-CA-C	7.50	121.97	108.69
1	A	125	SER	N-CA-C	7.45	119.64	108.31
1	D	190	ARG	CA-C-O	-6.92	109.04	120.80
1	A	177	GLN	CB-CA-C	-6.85	102.17	110.94
1	A	166	GLY	N-CA-C	6.70	121.15	110.90
1	C	70	LEU	N-CA-C	6.68	119.22	109.07
1	C	48	VAL	CB-CA-C	-6.67	100.90	110.83
1	E	88	LEU	N-CA-C	6.63	118.31	107.23
1	E	239	TYR	N-CA-C	-6.50	98.60	109.07
1	A	67	ILE	N-CA-C	6.49	117.22	107.80
1	A	48	VAL	CB-CA-C	-6.49	101.83	110.98
1	F	200	GLU	N-CA-C	-6.45	103.74	112.26
1	F	241	ILE	N-CA-C	-6.27	103.12	110.21
1	F	134	ARG	N-CA-C	6.24	118.16	111.36
1	D	65	ASN	N-CA-C	6.23	118.97	109.62
1	B	125	SER	CB-CA-C	-6.22	109.39	116.54
1	F	100	THR	N-CA-C	6.22	119.00	107.99
1	D	125	SER	CB-CA-C	-6.15	109.49	116.63
1	A	31	ASN	CA-C-N	-6.14	113.48	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASN	C-N-CA	-6.14	113.48	119.87
1	D	66	SER	N-CA-C	6.07	119.03	110.23
1	F	117	LYS	N-CA-C	-5.95	102.68	110.53
1	E	117	LYS	N-CA-C	-5.94	102.12	110.50
1	F	207	PHE	N-CA-C	5.89	117.74	108.96
1	C	113	GLU	N-CA-C	5.84	117.96	108.26
1	E	100	THR	N-CA-C	5.84	118.42	108.02
1	C	1	MET	CG-SD-CE	5.84	113.75	100.90
1	B	128	ILE	N-CA-C	5.82	115.36	108.96
1	E	200	GLU	N-CA-C	-5.81	106.19	113.28
1	B	118	LEU	N-CA-C	5.76	118.30	108.90
1	B	125	SER	N-CA-C	5.72	117.01	108.31
1	A	132	ASP	CA-C-N	-5.64	115.10	123.11
1	A	132	ASP	C-N-CA	-5.64	115.10	123.11
1	E	31	ASN	CA-C-N	-5.61	113.89	120.12
1	E	31	ASN	C-N-CA	-5.61	113.89	120.12
1	D	195	VAL	N-CA-C	5.59	116.26	108.89
1	E	63	GLY	N-CA-C	-5.54	106.09	112.73
1	C	134	ARG	CB-CA-C	-5.54	110.21	116.63
1	C	184	ALA	N-CA-C	5.49	119.55	111.04
1	C	147	ILE	N-CA-C	5.47	115.67	110.42
1	B	241	ILE	CB-CA-C	-5.46	102.33	111.29
1	F	105	ASN	CA-C-N	-5.44	113.01	119.05
1	F	105	ASN	C-N-CA	-5.44	113.01	119.05
1	B	147	ILE	N-CA-C	5.40	116.78	110.62
1	B	156	ASP	N-CA-C	-5.40	105.39	112.41
1	E	134	ARG	N-CA-C	5.38	117.15	111.28
1	D	105	ASN	CA-C-N	-5.36	113.10	119.05
1	D	105	ASN	C-N-CA	-5.36	113.10	119.05
1	D	70	LEU	N-CA-C	5.34	116.96	108.79
1	E	66	SER	N-CA-C	5.32	117.16	110.24
1	B	135	SER	N-CA-C	5.31	118.72	110.17
1	C	126	MET	CB-CA-C	-5.31	102.60	110.62
1	B	39	ALA	N-CA-C	5.25	117.23	108.99
1	A	137	VAL	N-CA-C	5.24	116.51	108.71
1	C	183	GLN	N-CA-C	5.18	117.89	109.24
1	F	27	ASN	N-CA-C	5.16	117.17	108.96
1	F	65	ASN	CB-CA-C	-5.15	103.74	111.73
1	C	104	GLU	CA-C-N	5.15	127.66	120.65
1	C	104	GLU	C-N-CA	5.15	127.66	120.65
1	E	58	VAL	N-CA-C	-5.15	107.28	112.17
1	A	29	ASP	CB-CA-C	-5.14	102.86	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	ASP	N-CA-C	5.12	118.79	112.24
1	B	58	VAL	N-CA-C	-5.11	106.09	110.74
1	E	59	LYS	N-CA-C	-5.10	100.98	108.79
1	B	143	GLU	N-CA-C	-5.05	105.46	110.97
1	C	242	ASP	CB-CA-C	-5.04	104.57	111.73

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLU	Peptide
1	B	134	ARG	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	1955	0	1948	77	0
1	B	1955	0	1948	105	0
1	C	1955	0	1948	125	0
1	D	1955	0	1948	140	0
1	E	1955	0	1948	121	0
1	F	1955	0	1948	165	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	F	3	0	0	1	0
All	All	11739	0	11688	724	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 31.

All (724) 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:E:241:ILE:HG21	1:E:244:VAL:HG22	1.27	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:LEU:HD23	1:F:246:TYR:CE1	1.82	1.14
1:B:131:MET:CG	1:B:132:ASP:HA	1.80	1.11
1:F:10:SER:HB3	1:F:14:ARG:NH1	1.66	1.09
1:D:134:ARG:HB3	1:D:200:GLU:HB2	1.28	1.08
1:E:50:MET:CE	1:E:52:LEU:HG	1.84	1.07
1:F:119:LEU:HB2	1:F:121:ILE:HG12	1.36	1.07
1:C:100:THR:HG22	1:C:115:GLN:HG2	1.35	1.06
1:F:10:SER:HB3	1:F:14:ARG:HH12	1.00	1.06
1:B:119:LEU:HA	1:B:120:GLU:HB2	1.37	1.06
1:F:130:GLU:HB3	1:F:131:MET:HG2	1.32	1.03
1:A:22:LEU:HD12	1:A:48:VAL:HG22	1.40	1.03
1:E:134:ARG:CZ	1:E:201:GLU:HG3	1.89	1.02
1:E:241:ILE:CG2	1:E:244:VAL:HG22	1.89	1.02
1:D:134:ARG:HG3	1:D:200:GLU:HG3	1.39	1.00
1:E:118:LEU:C	1:E:119:LEU:HD23	1.85	1.00
1:B:40:MET:HG3	1:B:47:LEU:HD23	1.43	1.00
1:F:122:GLU:OE2	1:F:122:GLU:N	1.94	1.00
1:A:130:GLU:HB2	1:A:131:MET:HB2	1.43	0.99
1:E:241:ILE:HG21	1:E:244:VAL:CG2	1.90	0.99
1:C:4:ALA:HB1	1:C:57:PHE:CD2	1.99	0.97
1:F:99:VAL:HG12	1:F:118:LEU:HD22	1.42	0.97
1:F:241:ILE:HD12	1:F:246:TYR:HA	1.46	0.95
1:B:134:ARG:HH11	1:B:201:GLU:HG3	1.28	0.95
1:F:130:GLU:HB3	1:F:131:MET:CG	1.95	0.95
1:D:31:ASN:HD22	1:D:65:ASN:HB2	1.27	0.95
1:D:50:MET:HE2	1:D:52:LEU:HG	1.49	0.95
1:D:19:ILE:HG22	1:D:48:VAL:HG11	1.49	0.94
1:F:164:LYS:HE3	1:F:199:MET:HE1	1.48	0.94
1:D:184:ALA:HB2	1:D:195:VAL:HG12	1.47	0.94
1:B:134:ARG:HA	1:B:200:GLU:HB3	1.50	0.94
1:C:131:MET:HB2	1:C:132:ASP:HB2	1.50	0.93
1:F:119:LEU:HB2	1:F:121:ILE:CG1	1.98	0.92
1:A:130:GLU:HB2	1:A:131:MET:CB	1.98	0.92
1:A:50:MET:HE3	1:A:52:LEU:HG	1.53	0.91
1:B:131:MET:CB	1:B:132:ASP:HA	1.99	0.91
1:F:10:SER:CB	1:F:14:ARG:HH12	1.83	0.91
1:A:86:ASP:OD2	1:A:110:ARG:NH2	2.04	0.91
1:E:50:MET:HE2	1:E:52:LEU:HG	1.51	0.90
1:D:237:VAL:HG22	1:D:249:TYR:HB2	1.55	0.89
1:D:134:ARG:HG2	1:D:134:ARG:HH11	1.35	0.89
1:F:105:ASN:OD1	1:F:107:GLU:N	2.05	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:MET:HE3	1:D:238:GLU:HB2	1.55	0.89
1:A:148:VAL:O	1:A:152:GLN:HG3	1.73	0.88
1:B:162:ILE:HG13	1:B:203:ILE:HG23	1.56	0.88
1:D:56:CYS:HB2	1:D:244:VAL:HB	1.56	0.88
1:F:5:GLN:HG2	1:F:58:VAL:CG2	2.04	0.88
1:B:119:LEU:CA	1:B:120:GLU:HB2	2.03	0.87
1:D:238:GLU:HG3	1:D:248:ARG:HD3	1.56	0.86
1:D:88:LEU:HD11	1:D:101:LEU:HD23	1.58	0.85
1:D:81:ILE:HD11	1:D:114:TYR:OH	1.75	0.84
1:F:16:VAL:HG21	1:F:79:LEU:CD1	2.06	0.84
1:C:22:LEU:HD12	1:C:48:VAL:CG2	2.08	0.84
1:B:131:MET:HG2	1:B:132:ASP:HA	1.58	0.84
1:F:104:GLU:HB3	1:F:108:LYS:HE2	1.59	0.84
1:B:134:ARG:HD3	1:B:201:GLU:HB2	1.60	0.83
1:F:16:VAL:HG21	1:F:79:LEU:HD12	1.57	0.83
1:B:134:ARG:NH1	1:B:201:GLU:HG3	1.92	0.83
1:F:51:LEU:HD23	1:F:246:TYR:HE1	1.37	0.83
1:A:132:ASP:HB3	1:A:134:ARG:HH11	1.41	0.83
1:C:132:ASP:OD1	1:C:133:TYR:N	2.12	0.83
1:B:31:ASN:HB3	1:B:32:PRO:CD	2.08	0.83
1:B:236:MET:HE3	1:B:238:GLU:HB2	1.61	0.82
1:D:49:HIS:ND1	1:D:128:ILE:HD12	1.94	0.82
1:F:241:ILE:HD12	1:F:246:TYR:CA	2.09	0.82
1:F:105:ASN:O	1:F:108:LYS:HE3	1.78	0.82
1:C:41:ASP:OD2	1:C:43:SER:HB2	1.79	0.82
1:A:144:PHE:HZ	1:A:212:MET:CE	1.93	0.81
1:E:150:ASP:O	1:E:153:VAL:HG22	1.81	0.81
1:F:119:LEU:CB	1:F:121:ILE:HG12	2.10	0.81
1:B:131:MET:HB3	1:B:132:ASP:HB3	1.60	0.81
1:D:51:LEU:HB3	1:D:246:TYR:CE1	2.15	0.81
1:E:56:CYS:HB2	1:E:244:VAL:HB	1.61	0.80
1:D:134:ARG:HB3	1:D:200:GLU:CB	2.11	0.80
1:B:118:LEU:HD12	1:B:118:LEU:O	1.82	0.80
1:F:27:ASN:ND2	1:F:121:ILE:HB	1.97	0.79
1:B:131:MET:CB	1:B:132:ASP:CA	2.61	0.79
1:B:131:MET:HB3	1:B:132:ASP:CA	2.13	0.79
1:A:40:MET:SD	1:A:44:HIS:HD2	2.04	0.78
1:E:139:LEU:HD11	1:E:144:PHE:HB2	1.64	0.78
1:F:50:MET:HE3	1:F:52:LEU:HG	1.64	0.78
1:C:236:MET:HE3	1:C:238:GLU:HB2	1.66	0.78
1:E:119:LEU:HD23	1:E:119:LEU:N	1.98	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ASP:O	1:F:96:SER:HB2	1.84	0.78
1:F:241:ILE:CD1	1:F:246:TYR:CA	2.62	0.78
1:E:22:LEU:HD12	1:E:48:VAL:CG2	2.15	0.77
1:F:31:ASN:HB3	1:F:65:ASN:ND2	1.98	0.77
1:A:132:ASP:HB3	1:A:134:ARG:NH1	1.99	0.77
1:A:159:THR:HA	1:A:206:SER:HB3	1.66	0.77
1:F:119:LEU:HA	1:F:120:GLU:HB3	1.67	0.77
1:A:22:LEU:CD1	1:A:48:VAL:HG22	2.15	0.76
1:E:236:MET:HE3	1:E:238:GLU:HB2	1.65	0.76
1:C:21:GLY:O	1:C:214:ILE:HD12	1.85	0.76
1:D:134:ARG:HD3	1:D:199:MET:HA	1.68	0.76
1:C:150:ASP:O	1:C:153:VAL:HG22	1.86	0.76
1:D:241:ILE:HG22	1:D:244:VAL:HG22	1.68	0.76
1:D:119:LEU:HD23	1:D:119:LEU:N	2.01	0.75
1:B:31:ASN:HB3	1:B:32:PRO:HD2	1.68	0.75
1:B:119:LEU:HD23	1:B:119:LEU:N	2.02	0.75
1:F:119:LEU:N	1:F:119:LEU:HD23	2.01	0.75
1:D:134:ARG:HG3	1:D:200:GLU:CG	2.16	0.74
1:E:70:LEU:HD23	1:E:99:VAL:HG11	1.69	0.74
1:F:164:LYS:HG2	1:F:199:MET:HE1	1.69	0.74
1:D:241:ILE:CG2	1:D:244:VAL:HG22	2.18	0.74
1:F:241:ILE:CD1	1:F:246:TYR:C	2.60	0.74
1:D:164:LYS:HG3	1:D:165:GLU:CG	2.17	0.74
1:D:118:LEU:C	1:D:119:LEU:HD23	2.12	0.74
1:F:27:ASN:HD21	1:F:121:ILE:HB	1.53	0.73
1:C:22:LEU:HD12	1:C:48:VAL:HG23	1.68	0.73
1:F:148:VAL:HG11	1:F:212:MET:HB3	1.69	0.73
1:E:246:TYR:CD2	1:E:248:ARG:HD2	2.22	0.73
1:D:74:SER:HB3	1:E:175:VAL:HG13	1.70	0.73
1:B:131:MET:HB3	1:B:132:ASP:CB	2.18	0.73
1:E:236:MET:HE3	1:E:248:ARG:HG2	1.70	0.73
1:D:164:LYS:HG3	1:D:165:GLU:HG2	1.71	0.73
1:F:130:GLU:CG	1:F:131:MET:HA	2.19	0.73
1:F:69:GLY:HA3	1:F:121:ILE:CD1	2.18	0.72
1:C:242:ASP:C	1:C:243:ASN:HD22	1.97	0.72
1:D:134:ARG:HG2	1:D:134:ARG:NH1	1.99	0.72
1:F:200:GLU:HG2	1:F:200:GLU:O	1.89	0.72
1:B:118:LEU:HD12	1:B:118:LEU:C	2.14	0.72
1:D:134:ARG:CG	1:D:200:GLU:HG3	2.20	0.72
1:F:2:LEU:C	1:F:2:LEU:HD23	2.15	0.71
1:F:154:PHE:O	1:F:173:GLY:HA3	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:GLU:HA	1:C:184:ALA:HB3	1.73	0.71
1:E:246:TYR:CD2	1:E:248:ARG:CD	2.74	0.71
1:F:25:GLU:OE1	1:F:119:LEU:HD12	1.90	0.71
1:D:49:HIS:ND1	1:D:128:ILE:CD1	2.53	0.70
1:F:69:GLY:CA	1:F:121:ILE:CD1	2.69	0.70
1:B:14:ARG:HD2	1:B:220:THR:HB	1.72	0.70
1:A:22:LEU:HD12	1:A:48:VAL:CG2	2.20	0.70
1:D:50:MET:CE	1:D:52:LEU:HG	2.20	0.70
1:F:119:LEU:HA	1:F:120:GLU:CB	2.21	0.70
1:A:75:LEU:HG	1:A:79:LEU:HD12	1.73	0.70
1:B:134:ARG:HD3	1:B:201:GLU:CG	2.22	0.69
1:B:48:VAL:HG13	1:B:249:TYR:CE1	2.27	0.69
1:C:201:GLU:HG2	1:C:202:PRO:HD2	1.73	0.69
1:A:110:ARG:HD3	1:D:143:GLU:OE1	1.91	0.69
1:A:216:ALA:HA	1:A:239:TYR:OH	1.93	0.69
1:F:207:PHE:HD2	1:F:251:LEU:HD23	1.58	0.69
1:E:134:ARG:NE	1:E:201:GLU:HG3	2.07	0.68
1:F:25:GLU:OE1	1:F:119:LEU:CD1	2.41	0.68
1:F:210:ARG:O	1:F:214:ILE:HG12	1.92	0.68
1:C:131:MET:CB	1:C:132:ASP:HB2	2.20	0.68
1:E:119:LEU:HA	1:E:120:GLU:HB2	1.74	0.68
1:B:134:ARG:HD3	1:B:201:GLU:CB	2.23	0.68
1:B:122:GLU:HG2	1:B:123:ALA:N	2.07	0.68
1:E:64:ARG:HH11	1:E:64:ARG:HB3	1.59	0.68
1:B:134:ARG:CD	1:B:201:GLU:HB2	2.23	0.68
1:C:133:TYR:HD2	1:C:134:ARG:H	1.41	0.68
1:A:14:ARG:HD2	1:A:220:THR:HB	1.74	0.68
1:B:94:ASP:O	1:B:95:ASP:OD1	2.11	0.68
1:B:3:GLU:HG3	1:B:91:ARG:HE	1.59	0.68
1:C:143:GLU:O	1:C:147:ILE:HG13	1.93	0.68
1:A:43:SER:OG	1:A:45:VAL:HG23	1.95	0.67
1:B:135:SER:OG	1:B:203:ILE:HG21	1.94	0.67
1:C:243:ASN:HD22	1:C:243:ASN:N	1.91	0.67
1:D:134:ARG:HB2	1:D:200:GLU:CD	2.19	0.67
1:E:64:ARG:HH11	1:E:64:ARG:CB	2.08	0.67
1:E:148:VAL:CG2	1:E:149:ARG:N	2.58	0.67
1:C:122:GLU:OE2	1:C:122:GLU:N	2.18	0.67
1:D:164:LYS:HA	1:D:199:MET:HE1	1.76	0.67
1:C:3:GLU:OE2	1:C:59:LYS:HE2	1.95	0.66
1:B:228:LYS:HD2	1:B:236:MET:HE2	1.77	0.66
1:C:64:ARG:CB	1:C:64:ARG:HH11	2.08	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HB3	1:D:61:GLN:NE2	2.10	0.66
1:F:99:VAL:CG1	1:F:118:LEU:HD22	2.20	0.66
1:A:139:LEU:HD11	1:A:144:PHE:HB2	1.77	0.66
1:A:134:ARG:O	1:A:200:GLU:HB2	1.95	0.66
1:F:69:GLY:O	1:F:118:LEU:HB2	1.95	0.66
1:F:70:LEU:N	1:F:121:ILE:HD11	2.10	0.66
1:E:125:SER:OG	1:E:126:MET:N	2.25	0.66
1:E:230:ALA:HB3	1:E:233:SER:HB2	1.78	0.66
1:B:25:GLU:HB2	1:B:121:ILE:CD1	2.26	0.66
1:C:43:SER:O	1:C:44:HIS:HB2	1.96	0.66
1:D:2:LEU:HG	1:D:3:GLU:N	2.10	0.66
1:C:241:ILE:HG22	1:C:241:ILE:O	1.95	0.65
1:D:22:LEU:HD12	1:D:48:VAL:CG2	2.26	0.65
1:F:187:VAL:HG11	1:F:196:GLU:OE2	1.96	0.65
1:D:43:SER:O	1:D:45:VAL:HG23	1.96	0.65
1:A:168:LYS:HD2	1:A:179:TYR:CD1	2.31	0.65
1:C:62:CYS:O	1:C:63:GLY:C	2.39	0.65
1:F:164:LYS:HG2	1:F:199:MET:CE	2.26	0.65
1:B:53:ARG:O	1:B:56:CYS:HB3	1.97	0.65
1:E:50:MET:HE1	1:E:52:LEU:HG	1.79	0.65
1:E:96:SER:O	1:E:97:ASP:HB3	1.94	0.65
1:B:92:HIS:HD2	1:B:98:VAL:O	1.80	0.65
1:B:125:SER:OG	1:B:126:MET:N	2.27	0.65
1:D:51:LEU:HD23	1:D:246:TYR:HE1	1.62	0.65
1:E:210:ARG:O	1:E:214:ILE:HG12	1.98	0.64
1:E:215:PHE:CD1	1:E:249:TYR:CG	2.85	0.64
1:B:87:SER:O	1:B:103:SER:HA	1.97	0.64
1:C:135:SER:OG	1:C:203:ILE:HG21	1.97	0.64
1:E:56:CYS:CB	1:E:244:VAL:HB	2.27	0.64
1:A:165:GLU:O	1:A:183:GLN:HA	1.98	0.63
1:E:148:VAL:CG2	1:E:149:ARG:H	2.10	0.63
1:C:154:PHE:O	1:C:173:GLY:HA3	1.98	0.63
1:F:5:GLN:O	1:F:57:PHE:HD2	1.82	0.63
1:F:159:THR:OG1	1:F:206:SER:HB3	1.98	0.63
1:B:40:MET:HG3	1:B:47:LEU:CD2	2.24	0.63
1:C:57:PHE:CD1	1:C:57:PHE:N	2.67	0.63
1:A:71:ASN:HB2	1:A:119:LEU:HD11	1.80	0.63
1:A:100:THR:HG22	1:A:115:GLN:HG2	1.80	0.63
1:C:15:LEU:HD13	1:C:50:MET:HE2	1.81	0.62
1:B:36:SER:HA	1:B:50:MET:O	1.99	0.62
1:B:25:GLU:HB2	1:B:121:ILE:HD13	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HB2	1:A:131:MET:CA	2.29	0.62
1:F:105:ASN:OD1	1:F:107:GLU:HB3	1.99	0.62
1:F:231:LYS:HE2	1:F:232:ASP:N	2.14	0.62
1:A:58:VAL:HG23	1:A:59:LYS:HG2	1.82	0.62
1:C:5:GLN:HB2	1:C:89:SER:OG	1.99	0.62
1:D:53:ARG:O	1:D:56:CYS:HB3	1.99	0.62
1:C:15:LEU:HD22	1:C:50:MET:HE2	1.82	0.61
1:A:133:TYR:CD2	1:A:228:LYS:HD3	2.36	0.61
1:F:69:GLY:HA3	1:F:121:ILE:HG13	1.81	0.61
1:B:2:LEU:O	1:B:91:ARG:HA	2.01	0.61
1:F:69:GLY:C	1:F:121:ILE:HD11	2.26	0.61
1:D:16:VAL:HG21	1:D:79:LEU:CD1	2.30	0.61
1:D:22:LEU:HD12	1:D:48:VAL:HG22	1.82	0.61
1:F:164:LYS:CE	1:F:199:MET:HE1	2.26	0.61
1:D:135:SER:OG	1:D:203:ILE:HG21	2.01	0.61
1:D:241:ILE:HG21	1:D:244:VAL:CG2	2.31	0.61
1:F:69:GLY:CA	1:F:121:ILE:HD11	2.31	0.60
1:E:154:PHE:O	1:E:173:GLY:HA3	2.01	0.60
1:F:241:ILE:CD1	1:F:246:TYR:HA	2.24	0.60
1:C:64:ARG:HH11	1:C:64:ARG:CG	2.14	0.60
1:D:105:ASN:HD22	1:D:110:ARG:H	1.48	0.60
1:A:105:ASN:HD22	1:A:110:ARG:N	1.98	0.60
1:B:119:LEU:HA	1:B:120:GLU:CB	2.24	0.60
1:D:105:ASN:ND2	1:D:109:THR:HG23	2.17	0.60
1:F:51:LEU:HD23	1:F:246:TYR:CZ	2.35	0.60
1:F:119:LEU:HB3	1:F:120:GLU:C	2.27	0.60
1:F:138:THR:HG22	1:F:224:ARG:HH21	1.67	0.60
1:A:133:TYR:HD2	1:A:228:LYS:HD3	1.65	0.59
1:E:148:VAL:HG23	1:E:149:ARG:N	2.15	0.59
1:B:105:ASN:HB3	1:B:108:LYS:H	1.67	0.59
1:D:54:ASP:CB	1:D:60:TYR:CD2	2.85	0.59
1:F:119:LEU:CA	1:F:120:GLU:HB3	2.32	0.59
1:C:93:ASP:O	1:C:96:SER:HB2	2.02	0.59
1:D:5:GLN:HB2	1:D:89:SER:OG	2.02	0.59
1:C:10:SER:HB3	1:C:14:ARG:HH12	1.67	0.59
1:C:131:MET:HB3	1:C:132:ASP:HA	1.84	0.59
1:D:134:ARG:CB	1:D:200:GLU:HB2	2.19	0.59
1:E:69:GLY:O	1:E:118:LEU:HB2	2.01	0.59
1:F:107:GLU:HG3	1:F:109:THR:HG23	1.85	0.59
1:D:54:ASP:HB3	1:D:60:TYR:CE2	2.37	0.59
1:D:54:ASP:HB2	1:D:60:TYR:HD2	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:THR:OG1	1:D:206:SER:HB3	2.03	0.58
1:E:119:LEU:CA	1:E:120:GLU:HB2	2.33	0.58
1:B:90:LEU:HD13	1:B:101:LEU:HD21	1.86	0.58
1:D:164:LYS:HG3	1:D:165:GLU:HG3	1.84	0.58
1:C:4:ALA:HB1	1:C:57:PHE:CE2	2.39	0.58
1:D:1:MET:HB3	1:D:61:GLN:HE21	1.66	0.58
1:C:122:GLU:H	1:C:122:GLU:CD	2.10	0.58
1:F:130:GLU:HG3	1:F:131:MET:HA	1.85	0.58
1:F:5:GLN:HG2	1:F:58:VAL:HG23	1.84	0.58
1:B:7:GLN:NE2	1:B:8:PHE:CZ	2.72	0.58
1:D:134:ARG:HA	1:D:134:ARG:NE	2.19	0.58
1:E:2:LEU:HD23	1:E:2:LEU:C	2.29	0.58
1:F:241:ILE:HD13	1:F:246:TYR:N	2.19	0.58
1:A:50:MET:HG2	1:A:51:LEU:N	2.19	0.57
1:A:179:TYR:CE2	1:E:113:GLU:HB3	2.40	0.57
1:B:49:HIS:ND1	1:B:128:ILE:HD11	2.20	0.57
1:D:134:ARG:CB	1:D:200:GLU:CD	2.77	0.57
1:F:50:MET:HB2	1:F:247:LEU:HD12	1.86	0.57
1:E:19:ILE:HD11	1:E:37:VAL:HG11	1.85	0.57
1:C:182:LEU:HB3	1:C:195:VAL:HG21	1.87	0.57
1:F:19:ILE:HD11	1:F:72:LEU:HD11	1.86	0.57
1:C:169:PHE:O	1:C:179:TYR:HA	2.04	0.57
1:D:107:GLU:HG2	1:D:109:THR:HG22	1.87	0.57
1:F:101:LEU:HD12	1:F:101:LEU:H	1.69	0.57
1:D:53:ARG:HB3	1:D:55:ASP:OD1	2.05	0.57
1:F:81:ILE:HD11	1:F:114:TYR:CZ	2.40	0.57
1:F:231:LYS:HE2	1:F:232:ASP:H	1.70	0.57
1:F:130:GLU:CB	1:F:131:MET:HA	2.35	0.56
1:F:156:ASP:OD1	1:F:156:ASP:N	2.38	0.56
1:C:15:LEU:HD22	1:C:50:MET:CE	2.35	0.56
1:E:246:TYR:CE2	1:E:248:ARG:NH1	2.73	0.56
1:F:5:GLN:HG2	1:F:58:VAL:HG22	1.86	0.56
1:A:105:ASN:HD22	1:A:110:ARG:H	1.54	0.56
1:C:243:ASN:N	1:C:243:ASN:ND2	2.50	0.56
1:D:105:ASN:HD22	1:D:110:ARG:N	2.03	0.56
1:F:50:MET:CE	1:F:52:LEU:HG	2.33	0.56
1:E:246:TYR:CD2	1:E:248:ARG:HD3	2.41	0.56
1:C:165:GLU:HA	1:C:184:ALA:CB	2.36	0.56
1:E:74:SER:O	1:E:78:VAL:HG23	2.06	0.56
1:F:148:VAL:CG1	1:F:212:MET:HB3	2.34	0.56
1:C:102:THR:HG23	1:C:113:GLU:HG3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:CD2	1:A:228:LYS:HB3	2.41	0.56
1:B:119:LEU:HB2	1:B:121:ILE:HG13	1.88	0.56
1:C:132:ASP:C	1:C:133:TYR:CD1	2.84	0.56
1:E:241:ILE:HD12	1:E:241:ILE:N	2.20	0.56
1:F:130:GLU:HG3	1:F:131:MET:HB3	1.88	0.55
1:B:37:VAL:HG23	1:B:50:MET:HE2	1.87	0.55
1:C:176:GLY:C	1:C:177:GLN:HG3	2.31	0.55
1:C:133:TYR:CD2	1:C:134:ARG:N	2.72	0.55
1:E:246:TYR:CE2	1:E:248:ARG:HD3	2.40	0.55
1:F:242:ASP:O	1:F:243:ASN:HB2	2.06	0.55
1:E:50:MET:CE	1:E:52:LEU:CG	2.73	0.55
1:B:172:SER:HB3	1:B:177:GLN:HG2	1.89	0.55
1:B:16:VAL:HG21	1:B:79:LEU:CD1	2.37	0.55
1:A:22:LEU:HD22	1:A:41:ASP:HB3	1.89	0.54
1:C:165:GLU:OE1	1:C:185:ALA:HB2	2.08	0.54
1:C:222:SER:HB2	1:C:240:GLY:O	2.07	0.54
1:D:210:ARG:O	1:D:214:ILE:HG12	2.07	0.54
1:F:119:LEU:CA	1:F:120:GLU:CB	2.85	0.54
1:B:172:SER:CB	1:B:177:GLN:HG2	2.38	0.54
1:D:31:ASN:ND2	1:D:65:ASN:HB2	2.09	0.54
1:D:71:ASN:OD1	1:D:73:ALA:HB3	2.07	0.54
1:B:130:GLU:OE1	1:B:130:GLU:N	2.41	0.54
1:C:131:MET:CB	1:C:132:ASP:CA	2.85	0.54
1:F:69:GLY:HA3	1:F:121:ILE:CG1	2.37	0.54
1:F:99:VAL:HG12	1:F:118:LEU:CD2	2.27	0.54
1:B:162:ILE:HG13	1:B:203:ILE:CG2	2.33	0.54
1:C:189:ASP:O	1:C:190:ARG:HB2	2.06	0.54
1:B:197:VAL:HG12	1:B:199:MET:HE2	1.89	0.54
1:C:75:LEU:HG	1:C:79:LEU:HD12	1.88	0.54
1:C:22:LEU:HD12	1:C:48:VAL:HG22	1.86	0.54
1:E:236:MET:CE	1:E:238:GLU:HB2	2.34	0.54
1:B:115:GLN:HB2	1:F:177:GLN:HB2	1.90	0.54
1:D:31:ASN:HD22	1:D:65:ASN:CB	2.10	0.54
1:D:40:MET:HG2	1:D:47:LEU:CD2	2.38	0.54
1:C:56:CYS:HB2	1:C:244:VAL:HB	1.89	0.54
1:E:68:LEU:HD22	1:E:92:HIS:CD2	2.43	0.54
1:A:75:LEU:HG	1:A:79:LEU:CD1	2.38	0.53
1:C:131:MET:CB	1:C:132:ASP:CB	2.85	0.53
1:E:148:VAL:HG22	1:E:149:ARG:H	1.71	0.53
1:C:4:ALA:HB1	1:C:57:PHE:HD2	1.65	0.53
1:C:90:LEU:HD11	1:C:99:VAL:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLU:HB3	1:D:217:LYS:HE2	1.90	0.53
1:E:6:VAL:HG22	1:E:7:GLN:N	2.22	0.53
1:C:39:ALA:O	1:C:47:LEU:HD23	2.09	0.53
1:E:236:MET:CE	1:E:248:ARG:HG2	2.38	0.53
1:D:166:GLY:HA3	1:D:182:LEU:O	2.08	0.53
1:D:105:ASN:ND2	1:D:109:THR:CG2	2.72	0.53
1:F:50:MET:HG2	1:F:51:LEU:N	2.21	0.53
1:C:57:PHE:N	1:C:57:PHE:HD1	2.06	0.53
1:C:108:LYS:CD	1:C:108:LYS:H	2.22	0.53
1:C:158:VAL:HB	1:C:209:LEU:HD21	1.90	0.53
1:D:241:ILE:CG2	1:D:244:VAL:CG2	2.86	0.53
1:C:30:CYS:SG	1:C:35:LEU:HD22	2.50	0.52
1:D:116:LEU:HD12	1:D:116:LEU:N	2.24	0.52
1:A:158:VAL:HB	1:A:209:LEU:HD21	1.91	0.52
1:E:133:TYR:CD1	1:E:133:TYR:C	2.87	0.52
1:F:227:LEU:HD22	1:F:237:VAL:HG12	1.91	0.52
1:B:103:SER:HB3	1:B:112:CYS:HB2	1.90	0.52
1:B:119:LEU:CB	1:B:120:GLU:HB2	2.38	0.52
1:D:227:LEU:HD22	1:D:237:VAL:HG12	1.91	0.52
1:C:238:GLU:HG3	1:C:248:ARG:HD2	1.91	0.52
1:E:50:MET:HB2	1:E:247:LEU:HD12	1.91	0.52
1:D:54:ASP:HB3	1:D:60:TYR:CD2	2.44	0.52
1:D:241:ILE:HG22	1:D:242:ASP:N	2.25	0.52
1:B:129:PRO:C	1:B:130:GLU:OE1	2.52	0.52
1:E:241:ILE:N	1:E:241:ILE:CD1	2.73	0.52
1:C:55:ASP:C	1:C:55:ASP:OD1	2.53	0.52
1:E:169:PHE:O	1:E:179:TYR:HA	2.10	0.52
1:E:246:TYR:HD2	1:E:248:ARG:CD	2.22	0.52
1:F:6:VAL:HG11	1:F:12:TRP:CD1	2.45	0.52
1:B:163:SER:O	1:B:164:LYS:C	2.53	0.52
1:C:209:LEU:O	1:C:210:ARG:C	2.53	0.52
1:D:246:TYR:HD2	1:D:248:ARG:HB2	1.74	0.52
1:E:89:SER:HB3	1:E:91:ARG:HH21	1.75	0.52
1:F:206:SER:C	1:F:207:PHE:CD1	2.88	0.52
1:C:15:LEU:HD11	1:C:52:LEU:HD21	1.92	0.51
1:C:32:PRO:HG3	1:C:62:CYS:O	2.10	0.51
1:D:70:LEU:HD23	1:D:99:VAL:HG11	1.92	0.51
1:F:47:LEU:O	1:F:249:TYR:HA	2.10	0.51
1:F:241:ILE:HD13	1:F:246:TYR:CA	2.41	0.51
1:F:30:CYS:SG	1:F:35:LEU:CD2	2.98	0.51
1:C:196:GLU:O	1:C:197:VAL:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LEU:C	1:E:118:LEU:HD12	2.35	0.51
1:E:119:LEU:HB3	1:E:120:GLU:HB2	1.92	0.51
1:F:130:GLU:HG2	1:F:131:MET:HE3	1.93	0.51
1:C:187:VAL:HG13	1:C:188:SER:N	2.24	0.51
1:B:43:SER:O	1:B:45:VAL:HG23	2.11	0.51
1:B:53:ARG:HB3	1:B:55:ASP:OD1	2.11	0.51
1:D:213:GLY:O	1:D:214:ILE:C	2.52	0.51
1:F:205:LEU:HD22	1:F:253:PRO:HB3	1.92	0.51
1:C:6:VAL:HG22	1:C:7:GLN:N	2.25	0.51
1:E:92:HIS:ND1	1:E:93:ASP:N	2.57	0.51
1:E:230:ALA:O	1:E:231:LYS:C	2.54	0.51
1:F:1:MET:N	1:F:94:ASP:OD2	2.43	0.51
1:C:187:VAL:O	1:C:188:SER:C	2.53	0.51
1:F:69:GLY:CA	1:F:121:ILE:HD12	2.39	0.51
1:B:105:ASN:HD22	1:B:110:ARG:H	1.58	0.51
1:C:27:ASN:HA	1:C:69:GLY:HA2	1.93	0.51
1:C:132:ASP:O	1:C:133:TYR:CD1	2.64	0.51
1:F:31:ASN:HB2	1:F:32:PRO:HD3	1.92	0.51
1:B:119:LEU:HB3	1:B:120:GLU:HB2	1.93	0.51
1:C:22:LEU:HD22	1:C:41:ASP:HB3	1.93	0.51
1:E:215:PHE:CE1	1:E:249:TYR:HB3	2.46	0.51
1:C:64:ARG:CG	1:C:64:ARG:NH1	2.73	0.50
1:A:139:LEU:HD23	1:A:139:LEU:H	1.76	0.50
1:C:5:GLN:O	1:C:57:PHE:HB3	2.11	0.50
1:E:6:VAL:HG11	1:E:12:TRP:CD1	2.47	0.50
1:A:144:PHE:HZ	1:A:212:MET:HE2	1.73	0.50
1:F:135:SER:OG	1:F:203:ILE:HG21	2.10	0.50
1:E:134:ARG:NH1	1:E:201:GLU:HG3	2.26	0.50
1:F:11:LEU:O	1:F:11:LEU:HD12	2.11	0.50
1:F:71:ASN:HB3	1:F:74:SER:OG	2.11	0.50
1:A:161:ALA:HB3	1:A:168:LYS:HB3	1.92	0.50
1:E:145:ALA:HA	1:E:216:ALA:HB1	1.93	0.50
1:C:105:ASN:HB3	1:C:108:LYS:HA	1.93	0.50
1:F:4:ALA:O	1:F:90:LEU:N	2.45	0.50
1:F:200:GLU:O	1:F:201:GLU:HG2	2.12	0.50
1:A:209:LEU:O	1:A:210:ARG:C	2.55	0.50
1:B:28:PHE:CE1	1:B:70:LEU:HD11	2.45	0.50
1:D:57:PHE:N	1:D:57:PHE:CD1	2.80	0.50
1:F:31:ASN:HB2	1:F:32:PRO:CD	2.42	0.50
1:F:130:GLU:CB	1:F:131:MET:CA	2.90	0.50
1:C:30:CYS:HB2	1:C:66:SER:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:O	1:C:214:ILE:HG12	2.13	0.49
1:D:14:ARG:HD2	1:D:220:THR:HB	1.93	0.49
1:F:87:SER:O	1:F:103:SER:HA	2.12	0.49
1:D:246:TYR:CE2	1:D:248:ARG:CZ	2.94	0.49
1:F:1:MET:H3	1:F:94:ASP:CG	2.19	0.49
1:C:201:GLU:HG2	1:C:202:PRO:CD	2.40	0.49
1:D:132:ASP:C	1:D:133:TYR:HD1	2.20	0.49
1:B:5:GLN:HB2	1:B:89:SER:OG	2.12	0.49
1:C:179:TYR:CE2	1:F:113:GLU:HB3	2.47	0.49
1:D:54:ASP:CB	1:D:60:TYR:HD2	2.24	0.49
1:E:246:TYR:HD2	1:E:248:ARG:HD2	1.72	0.49
1:F:5:GLN:O	1:F:57:PHE:CD2	2.63	0.49
1:D:134:ARG:CG	1:D:200:GLU:CG	2.86	0.49
1:E:59:LYS:O	1:E:60:TYR:HB2	2.12	0.49
1:F:143:GLU:O	1:F:147:ILE:HG13	2.12	0.49
1:A:7:GLN:O	1:A:87:SER:HA	2.13	0.49
1:B:154:PHE:HB3	1:B:172:SER:HA	1.93	0.49
1:C:124:GLU:HG2	1:C:125:SER:N	2.28	0.49
1:F:28:PHE:CD1	1:F:37:VAL:HG22	2.48	0.49
1:F:246:TYR:CE2	1:F:248:ARG:CZ	2.95	0.49
1:B:57:PHE:CD1	1:B:57:PHE:N	2.80	0.49
1:E:188:SER:OG	1:E:189:ASP:HB3	2.12	0.49
1:D:19:ILE:CG2	1:D:48:VAL:HG11	2.34	0.49
1:C:100:THR:CG2	1:C:115:GLN:HG2	2.25	0.49
1:D:211:PHE:HA	1:D:214:ILE:HG12	1.94	0.49
1:D:215:PHE:CD1	1:D:249:TYR:CD1	3.01	0.49
1:D:230:ALA:O	1:D:231:LYS:C	2.55	0.49
1:F:119:LEU:HB3	1:F:120:GLU:HB3	1.93	0.49
1:F:203:ILE:CG1	1:F:204:THR:N	2.75	0.48
1:E:140:ASN:HB3	1:E:143:GLU:HB3	1.95	0.48
1:C:15:LEU:CD1	1:C:50:MET:HE2	2.43	0.48
1:E:60:TYR:HE1	1:E:62:CYS:HB2	1.78	0.48
1:F:98:VAL:HG13	1:F:116:LEU:O	2.12	0.48
1:D:133:TYR:CD2	1:D:230:ALA:HB1	2.49	0.48
1:E:67:ILE:O	1:E:68:LEU:HD23	2.12	0.48
1:F:30:CYS:SG	1:F:35:LEU:HD21	2.53	0.48
1:B:58:VAL:HG23	1:B:59:LYS:H	1.78	0.48
1:E:15:LEU:O	1:E:19:ILE:HG22	2.13	0.48
1:F:1:MET:N	1:F:94:ASP:CG	2.71	0.48
1:F:162:ILE:HD11	1:F:229:PHE:CE1	2.48	0.48
1:B:216:ALA:HA	1:B:239:TYR:OH	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:CYS:HB3	1:C:249:TYR:OH	2.13	0.48
1:D:124:GLU:OE1	1:D:124:GLU:HA	2.12	0.48
1:D:134:ARG:CB	1:D:200:GLU:CG	2.91	0.48
1:A:201:GLU:HB3	1:A:202:PRO:HD2	1.95	0.48
1:D:236:MET:SD	1:D:248:ARG:HD2	2.53	0.48
1:F:207:PHE:CD2	1:F:251:LEU:HD23	2.45	0.48
1:C:118:LEU:HD12	1:C:118:LEU:H	1.78	0.48
1:E:64:ARG:NH1	1:E:64:ARG:HA	2.29	0.48
1:D:45:VAL:HG12	1:D:45:VAL:O	2.12	0.48
1:E:241:ILE:HG22	1:E:244:VAL:HG22	1.84	0.48
1:A:53:ARG:O	1:A:56:CYS:HB3	2.14	0.47
1:A:102:THR:HG23	1:A:113:GLU:HG3	1.95	0.47
1:D:56:CYS:CB	1:D:244:VAL:HB	2.38	0.47
1:C:158:VAL:HG13	1:C:158:VAL:O	2.14	0.47
1:C:236:MET:HE1	1:C:248:ARG:HH11	1.77	0.47
1:D:16:VAL:HG21	1:D:79:LEU:HD11	1.96	0.47
1:D:199:MET:HG2	1:D:200:GLU:N	2.29	0.47
1:D:203:ILE:HG23	1:D:203:ILE:O	2.14	0.47
1:E:143:GLU:O	1:E:147:ILE:HG13	2.15	0.47
1:B:16:VAL:HG21	1:B:79:LEU:HD12	1.97	0.47
1:D:93:ASP:O	1:D:94:ASP:C	2.58	0.47
1:D:164:LYS:CG	1:D:165:GLU:HG3	2.43	0.47
1:E:128:ILE:HG22	1:E:130:GLU:HG3	1.95	0.47
1:B:15:LEU:CD1	1:B:50:MET:SD	3.03	0.47
1:B:98:VAL:HG12	1:B:99:VAL:N	2.29	0.47
1:C:10:SER:HB3	1:C:14:ARG:NH1	2.30	0.47
1:C:99:VAL:HG12	1:C:118:LEU:HD23	1.96	0.47
1:C:144:PHE:O	1:C:148:VAL:HG13	2.14	0.47
1:E:6:VAL:CG2	1:E:7:GLN:N	2.78	0.47
1:E:40:MET:HG2	1:E:47:LEU:HD22	1.97	0.47
1:E:207:PHE:CE2	1:E:235:CYS:SG	3.08	0.47
1:F:130:GLU:HB3	1:F:131:MET:CB	2.44	0.47
1:A:126:MET:HG3	1:A:127:GLY:H	1.80	0.47
1:A:197:VAL:HG12	1:A:198:THR:N	2.29	0.47
1:B:227:LEU:HA	1:B:236:MET:O	2.15	0.47
1:C:43:SER:HB2	1:C:45:VAL:HG12	1.96	0.47
1:D:218:GLY:O	1:D:221:LEU:HB2	2.15	0.47
1:E:14:ARG:HD2	1:E:220:THR:HB	1.97	0.47
1:E:67:ILE:C	1:E:68:LEU:HD23	2.40	0.47
1:E:118:LEU:O	1:E:119:LEU:HD23	2.12	0.47
1:F:15:LEU:O	1:F:19:ILE:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:TYR:CD1	1:C:61:GLN:N	2.83	0.47
1:C:131:MET:HB3	1:C:132:ASP:CA	2.44	0.47
1:F:19:ILE:HD11	1:F:72:LEU:CD1	2.45	0.47
1:F:130:GLU:CG	1:F:131:MET:HE3	2.45	0.47
1:A:160:ILE:HG12	1:A:169:PHE:CD1	2.50	0.47
1:C:106:PRO:O	1:C:107:GLU:CD	2.57	0.47
1:F:16:VAL:CG2	1:F:79:LEU:CD1	2.88	0.47
1:F:243:ASN:HD22	1:F:243:ASN:HA	1.57	0.46
1:B:229:PHE:N	1:B:229:PHE:CD1	2.84	0.46
1:D:54:ASP:HB2	1:D:60:TYR:CD2	2.48	0.46
1:D:69:GLY:O	1:D:118:LEU:HB2	2.15	0.46
1:B:228:LYS:HD2	1:B:236:MET:CE	2.43	0.46
1:B:231:LYS:O	1:B:232:ASP:HB2	2.13	0.46
1:D:130:GLU:OE2	1:D:130:GLU:N	2.48	0.46
1:F:164:LYS:CG	1:F:199:MET:HE1	2.44	0.46
1:B:177:GLN:O	1:C:114:TYR:HA	2.16	0.46
1:F:4:ALA:O	1:F:89:SER:HA	2.16	0.46
1:A:22:LEU:CD1	1:A:48:VAL:CG2	2.88	0.46
1:B:82:VAL:HG11	1:B:88:LEU:HD13	1.98	0.46
1:A:47:LEU:HD23	1:A:250:TYR:CD1	2.50	0.46
1:A:138:THR:HG23	1:A:226:THR:OG1	2.15	0.46
1:F:153:VAL:O	1:F:175:VAL:HG21	2.15	0.46
1:C:28:PHE:CD1	1:C:37:VAL:HG22	2.51	0.46
1:D:40:MET:HG2	1:D:47:LEU:HD22	1.98	0.46
1:C:237:VAL:HG22	1:C:249:TYR:HB2	1.97	0.46
1:D:6:VAL:HG22	1:D:7:GLN:N	2.30	0.46
1:F:94:ASP:OD1	1:F:94:ASP:N	2.47	0.46
1:C:145:ALA:HA	1:C:216:ALA:HB1	1.98	0.46
1:E:78:VAL:O	1:E:82:VAL:HG23	2.16	0.46
1:E:90:LEU:HD12	1:E:90:LEU:HA	1.62	0.46
1:C:135:SER:OG	1:C:203:ILE:CG2	2.64	0.45
1:D:241:ILE:CG2	1:D:242:ASP:N	2.79	0.45
1:E:57:PHE:CD1	1:E:57:PHE:N	2.82	0.45
1:F:212:MET:O	1:F:215:PHE:HB2	2.16	0.45
1:B:15:LEU:HD13	1:B:50:MET:SD	2.57	0.45
1:E:60:TYR:CE1	1:E:62:CYS:HB2	2.51	0.45
1:E:237:VAL:HG22	1:E:249:TYR:HB2	1.99	0.45
1:B:182:LEU:HD23	1:C:110:ARG:HB2	1.97	0.45
1:E:2:LEU:HD23	1:E:3:GLU:N	2.30	0.45
1:F:119:LEU:HB2	1:F:121:ILE:HG13	1.91	0.45
1:A:140:ASN:HB3	1:A:143:GLU:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PHE:CD1	1:B:28:PHE:N	2.82	0.45
1:D:216:ALA:HA	1:D:239:TYR:OH	2.17	0.45
1:F:130:GLU:HG3	1:F:131:MET:CB	2.46	0.45
1:A:17:GLU:O	1:A:18:CYS:C	2.60	0.45
1:B:233:SER:O	1:B:234:PRO:C	2.58	0.45
1:C:87:SER:O	1:C:103:SER:HA	2.16	0.45
1:E:22:LEU:HD12	1:E:48:VAL:HG23	1.95	0.45
1:A:55:ASP:OD1	1:A:55:ASP:N	2.48	0.45
1:D:225:VAL:HG21	1:D:239:TYR:CZ	2.52	0.45
1:F:21:GLY:O	1:F:214:ILE:HD12	2.17	0.45
1:F:35:LEU:HD12	1:F:57:PHE:CZ	2.52	0.45
1:A:2:LEU:O	1:A:91:ARG:HA	2.17	0.45
1:A:46:ALA:HA	1:A:250:TYR:O	2.16	0.45
1:B:131:MET:HG2	1:B:132:ASP:CA	2.38	0.45
1:C:227:LEU:HB2	1:C:229:PHE:HE1	1.81	0.45
1:E:216:ALA:HA	1:E:239:TYR:OH	2.16	0.45
1:C:217:LYS:O	1:C:220:THR:HG23	2.17	0.45
1:C:246:TYR:CD1	1:C:248:ARG:NE	2.85	0.45
1:D:11:LEU:HG	1:D:15:LEU:HD12	1.98	0.45
1:D:126:MET:C	1:D:127:GLY:O	2.58	0.45
1:F:159:THR:HG1	1:F:206:SER:HB3	1.83	0.45
1:E:60:TYR:CD1	1:E:61:GLN:N	2.84	0.44
1:A:12:TRP:O	1:A:16:VAL:HG23	2.16	0.44
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.83	0.44
1:B:51:LEU:HB3	1:B:246:TYR:CE2	2.51	0.44
1:E:36:SER:HA	1:E:50:MET:O	2.18	0.44
1:F:94:ASP:CB	2:F:303:HOH:O	2.65	0.44
1:F:241:ILE:HG22	1:F:242:ASP:N	2.32	0.44
1:E:164:LYS:HA	1:E:199:MET:HE1	1.99	0.44
1:F:119:LEU:CB	1:F:120:GLU:HB3	2.47	0.44
1:F:241:ILE:HD12	1:F:246:TYR:C	2.36	0.44
1:A:130:GLU:CB	1:A:131:MET:CA	2.92	0.44
1:B:199:MET:HG3	1:B:201:GLU:O	2.17	0.44
1:B:207:PHE:CZ	1:B:235:CYS:HB3	2.52	0.44
1:D:12:TRP:O	1:D:16:VAL:HG23	2.17	0.44
1:D:40:MET:CE	1:D:44:HIS:HA	2.47	0.44
1:E:16:VAL:HA	1:E:19:ILE:HG23	2.00	0.44
1:C:187:VAL:CG1	1:C:188:SER:N	2.80	0.44
1:E:16:VAL:O	1:E:20:ASN:HB2	2.16	0.44
1:E:242:ASP:OD1	1:E:242:ASP:N	2.50	0.44
1:A:78:VAL:O	1:A:81:ILE:HG12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:O	1:B:51:LEU:HD12	2.18	0.44
1:B:134:ARG:HD3	1:B:201:GLU:HG3	1.97	0.44
1:D:133:TYR:CD1	1:D:133:TYR:N	2.85	0.44
1:B:230:ALA:HB3	1:B:233:SER:HB3	1.99	0.44
1:C:189:ASP:O	1:C:190:ARG:HD3	2.17	0.44
1:E:246:TYR:CE2	1:E:248:ARG:CD	3.00	0.44
1:A:40:MET:HG3	1:A:47:LEU:HD12	1.99	0.44
1:A:48:VAL:HG13	1:A:249:TYR:CE1	2.53	0.44
1:B:160:ILE:O	1:B:204:THR:HA	2.18	0.44
1:C:15:LEU:CD2	1:C:50:MET:HE2	2.47	0.44
1:D:179:TYR:CD1	1:D:179:TYR:C	2.96	0.44
1:E:50:MET:HE2	1:E:52:LEU:CG	2.36	0.44
1:E:70:LEU:CD2	1:E:99:VAL:HG11	2.41	0.44
1:F:61:GLN:HE21	1:F:61:GLN:HB3	1.58	0.44
1:A:144:PHE:CZ	1:A:212:MET:CE	2.85	0.43
1:C:7:GLN:NE2	1:C:8:PHE:CE1	2.86	0.43
1:C:132:ASP:HB3	1:C:133:TYR:HD1	1.83	0.43
1:F:98:VAL:HA	1:F:118:LEU:CD2	2.47	0.43
1:A:71:ASN:OD1	1:A:73:ALA:HB3	2.18	0.43
1:C:64:ARG:NH1	1:C:64:ARG:HG2	2.32	0.43
1:D:215:PHE:CD1	1:D:249:TYR:CG	3.07	0.43
1:E:105:ASN:OD1	1:E:109:THR:HG23	2.18	0.43
1:A:144:PHE:CZ	1:A:212:MET:HE2	2.51	0.43
1:C:180:THR:HG22	1:C:182:LEU:HD12	2.00	0.43
1:E:148:VAL:HG21	1:E:213:GLY:HA2	1.99	0.43
1:E:165:GLU:H	1:E:199:MET:HE1	1.83	0.43
1:F:74:SER:O	1:F:78:VAL:HG23	2.18	0.43
1:B:28:PHE:CE1	1:B:70:LEU:CD1	3.02	0.43
1:E:38:GLN:HE21	1:E:38:GLN:HB2	1.61	0.43
1:B:55:ASP:OD1	1:B:55:ASP:N	2.52	0.43
1:F:186:GLY:HA3	1:F:187:VAL:HG13	1.99	0.43
1:D:47:LEU:HB3	1:D:250:TYR:HB2	2.01	0.43
1:F:79:LEU:HD23	1:F:79:LEU:HA	1.80	0.43
1:A:144:PHE:O	1:A:148:VAL:HG13	2.18	0.43
1:D:154:PHE:O	1:D:173:GLY:HA3	2.18	0.43
1:E:119:LEU:CB	1:E:120:GLU:HB2	2.49	0.43
1:F:215:PHE:CE1	1:F:249:TYR:HB3	2.53	0.43
1:D:222:SER:HB2	1:D:240:GLY:O	2.18	0.43
1:E:6:VAL:CG2	1:E:7:GLN:H	2.32	0.43
1:F:241:ILE:HD12	1:F:241:ILE:H	1.83	0.43
1:A:80:LYS:HD3	1:A:80:LYS:HA	1.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLY:HA2	1:B:183:GLN:HA	2.01	0.43
1:F:122:GLU:N	1:F:122:GLU:CD	2.73	0.43
1:C:133:TYR:O	1:C:134:ARG:HB2	2.18	0.43
1:D:105:ASN:ND2	1:D:110:ARG:HB3	2.34	0.43
1:D:153:VAL:O	1:D:175:VAL:HG21	2.17	0.43
1:F:246:TYR:CZ	1:F:248:ARG:NH2	2.87	0.43
1:B:210:ARG:O	1:B:214:ILE:HG13	2.18	0.42
1:C:196:GLU:OE2	1:C:196:GLU:N	2.52	0.42
1:D:233:SER:O	1:D:253:PRO:HG3	2.19	0.42
1:D:237:VAL:CG2	1:D:249:TYR:HB2	2.37	0.42
1:F:30:CYS:O	1:F:65:ASN:HA	2.19	0.42
1:C:124:GLU:O	1:C:125:SER:HB2	2.20	0.42
1:C:139:LEU:HD23	1:C:139:LEU:N	2.33	0.42
1:D:3:GLU:HA	1:D:90:LEU:O	2.19	0.42
1:D:107:GLU:OE1	1:D:107:GLU:N	2.43	0.42
1:D:148:VAL:HG23	1:D:149:ARG:N	2.34	0.42
1:D:246:TYR:CE2	1:D:248:ARG:NH2	2.87	0.42
1:D:246:TYR:CZ	1:D:248:ARG:NH2	2.87	0.42
1:C:62:CYS:O	1:C:63:GLY:O	2.36	0.42
1:C:131:MET:CB	1:C:132:ASP:HA	2.45	0.42
1:D:132:ASP:C	1:D:133:TYR:CD1	2.97	0.42
1:D:135:SER:HA	1:D:199:MET:HB2	2.00	0.42
1:D:246:TYR:CD2	1:D:248:ARG:HB2	2.53	0.42
1:B:50:MET:HE2	1:B:50:MET:HB3	1.98	0.42
1:C:60:TYR:HE1	1:C:62:CYS:HB2	1.85	0.42
1:D:87:SER:O	1:D:103:SER:HA	2.19	0.42
1:D:156:ASP:OD1	1:D:156:ASP:N	2.51	0.42
1:E:31:ASN:C	1:E:33:GLY:N	2.76	0.42
1:F:83:ASP:O	1:F:84:SER:C	2.61	0.42
1:E:38:GLN:O	1:E:39:ALA:HB2	2.19	0.42
1:E:53:ARG:O	1:E:56:CYS:HB3	2.20	0.42
1:F:69:GLY:HA2	1:F:121:ILE:HD12	2.02	0.42
1:F:101:LEU:HD12	1:F:101:LEU:N	2.32	0.42
1:B:1:MET:HE2	1:B:1:MET:HB2	1.71	0.42
1:C:132:ASP:O	1:C:133:TYR:CG	2.72	0.42
1:B:92:HIS:CD2	1:B:98:VAL:O	2.67	0.42
1:D:134:ARG:HD3	1:D:134:ARG:C	2.45	0.42
1:E:236:MET:CE	1:E:238:GLU:OE1	2.68	0.42
1:F:133:TYR:CG	1:F:228:LYS:HB3	2.55	0.42
1:A:6:VAL:HG22	1:A:7:GLN:N	2.34	0.42
1:B:175:VAL:HG13	1:C:74:SER:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:GLU:HB3	1:E:217:LYS:HE2	2.01	0.42
1:A:12:TRP:CD1	1:A:88:LEU:HD23	2.54	0.42
1:C:19:ILE:HG21	1:C:19:ILE:HD13	1.51	0.42
1:D:24:ASN:OD1	1:D:24:ASN:N	2.48	0.42
1:D:234:PRO:HA	1:D:251:LEU:O	2.19	0.42
1:F:51:LEU:CD2	1:F:246:TYR:HE1	2.18	0.42
1:D:19:ILE:HG23	1:D:19:ILE:HD13	1.66	0.42
1:A:147:ILE:CD1	1:A:182:LEU:HD11	2.50	0.41
1:A:147:ILE:O	1:A:151:MET:HG2	2.20	0.41
1:B:138:THR:HA	1:B:225:VAL:O	2.19	0.41
1:C:166:GLY:HA2	1:C:182:LEU:O	2.20	0.41
1:F:98:VAL:HA	1:F:118:LEU:HD23	2.02	0.41
1:F:104:GLU:HB3	1:F:108:LYS:CE	2.42	0.41
1:C:146:LYS:HD3	1:C:150:ASP:OD2	2.20	0.41
1:D:13:LYS:HD2	1:D:82:VAL:O	2.20	0.41
1:F:215:PHE:CD1	1:F:249:TYR:CG	3.08	0.41
1:D:118:LEU:CA	1:D:119:LEU:HD23	2.49	0.41
1:E:15:LEU:CD2	1:E:247:LEU:HD13	2.50	0.41
1:F:17:GLU:HB3	1:F:217:LYS:HE3	2.01	0.41
1:C:1:MET:HE2	1:C:1:MET:HB2	1.89	0.41
1:C:22:LEU:CD1	1:C:48:VAL:HG23	2.45	0.41
1:F:236:MET:SD	1:F:248:ARG:HG2	2.61	0.41
1:A:115:GLN:HB2	1:D:177:GLN:HG3	2.02	0.41
1:A:217:LYS:C	1:A:219:SER:H	2.27	0.41
1:E:140:ASN:HB3	1:E:143:GLU:CB	2.51	0.41
1:E:206:SER:C	1:E:207:PHE:CD1	2.99	0.41
1:E:228:LYS:C	1:E:229:PHE:CD1	2.99	0.41
1:F:5:GLN:HA	1:F:89:SER:HA	2.02	0.41
1:A:135:SER:OG	1:A:203:ILE:HG21	2.20	0.41
1:C:118:LEU:HD12	1:C:118:LEU:N	2.33	0.41
1:D:134:ARG:HH11	1:D:134:ARG:CG	2.14	0.41
1:A:131:MET:O	1:A:132:ASP:C	2.63	0.41
1:A:188:SER:HA	1:A:189:ASP:HA	1.72	0.41
1:B:134:ARG:HA	1:B:200:GLU:CB	2.36	0.41
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.84	0.41
1:C:216:ALA:C	1:C:218:GLY:N	2.78	0.41
1:D:19:ILE:HD12	1:D:19:ILE:HG21	1.70	0.41
1:E:68:LEU:HD13	1:E:92:HIS:HD2	1.86	0.41
1:B:37:VAL:HG23	1:B:50:MET:CE	2.51	0.41
1:B:83:ASP:O	1:B:84:SER:C	2.63	0.41
1:B:119:LEU:HB3	1:B:120:GLU:CB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ASN:HB3	1:E:108:LYS:N	2.36	0.41
1:E:153:VAL:HG23	1:E:154:PHE:CD1	2.56	0.41
1:F:132:ASP:OD1	1:F:133:TYR:N	2.54	0.41
1:F:209:LEU:HD23	1:F:209:LEU:HA	1.80	0.41
1:B:22:LEU:HD23	1:B:23:VAL:HG13	2.02	0.41
1:E:89:SER:CB	1:E:91:ARG:HH21	2.33	0.41
1:E:216:ALA:C	1:E:218:GLY:N	2.78	0.41
1:E:235:CYS:O	1:E:250:TYR:HA	2.21	0.41
1:F:5:GLN:HE21	1:F:58:VAL:HG21	1.85	0.41
1:F:27:ASN:OD1	1:F:67:ILE:HG22	2.20	0.41
1:F:138:THR:HG1	1:F:226:THR:HG23	1.86	0.41
1:F:186:GLY:HA2	1:F:187:VAL:HA	1.91	0.41
1:D:225:VAL:CG2	1:D:239:TYR:CE2	3.04	0.40
1:E:209:LEU:O	1:E:210:ARG:C	2.62	0.40
1:A:25:GLU:HB2	1:A:121:ILE:HD11	2.04	0.40
1:D:246:TYR:CD2	1:D:248:ARG:CZ	3.05	0.40
1:E:147:ILE:HG13	1:E:147:ILE:H	1.60	0.40
1:B:134:ARG:HH11	1:B:201:GLU:CG	2.12	0.40
1:F:2:LEU:HD23	1:F:2:LEU:O	2.20	0.40
1:F:165:GLU:N	1:F:165:GLU:OE2	2.54	0.40
1:D:131:MET:HB3	1:D:133:TYR:HE1	1.86	0.40
1:F:1:MET:HE2	1:F:1:MET:HB3	1.76	0.40
1:F:216:ALA:HA	1:F:239:TYR:OH	2.21	0.40
1:A:201:GLU:CB	1:A:202:PRO:HD2	2.51	0.40
1:D:81:ILE:HD11	1:D:114:TYR:CZ	2.56	0.40
1:E:222:SER:OG	1:E:224:ARG:O	2.36	0.40

There are no symmetry-related clashes.

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	249/259 (96%)	228 (92%)	21 (8%)	0	100	100
1	B	249/259 (96%)	227 (91%)	22 (9%)	0	100	100
1	C	249/259 (96%)	216 (87%)	32 (13%)	1 (0%)	30	62
1	D	249/259 (96%)	221 (89%)	26 (10%)	2 (1%)	16	50
1	E	249/259 (96%)	217 (87%)	29 (12%)	3 (1%)	10	42
1	F	249/259 (96%)	219 (88%)	29 (12%)	1 (0%)	30	62
All	All	1494/1554 (96%)	1328 (89%)	159 (11%)	7 (0%)	24	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	63	GLY
1	D	127	GLY
1	E	54	ASP
1	D	95	ASP
1	E	2	LEU
1	F	63	GLY
1	E	175	VAL

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	220/225 (98%)	168 (76%)	52 (24%)	1	4
1	B	220/225 (98%)	177 (80%)	43 (20%)	1	8
1	C	220/225 (98%)	166 (76%)	54 (24%)	1	3
1	D	220/225 (98%)	170 (77%)	50 (23%)	1	5
1	E	220/225 (98%)	168 (76%)	52 (24%)	1	4
1	F	220/225 (98%)	157 (71%)	63 (29%)	0	2
All	All	1320/1350 (98%)	1006 (76%)	314 (24%)	1	4

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	GLN
1	A	13	LYS
1	A	15	LEU
1	A	19	ILE
1	A	29	ASP
1	A	36	SER
1	A	40	MET
1	A	41	ASP
1	A	45	VAL
1	A	48	VAL
1	A	50	MET
1	A	53	ARG
1	A	54	ASP
1	A	56	CYS
1	A	64	ARG
1	A	65	ASN
1	A	74	SER
1	A	80	LYS
1	A	84	SER
1	A	89	SER
1	A	97	ASP
1	A	100	THR
1	A	102	THR
1	A	103	SER
1	A	107	GLU
1	A	109	THR
1	A	111	LYS
1	A	116	LEU
1	A	120	GLU
1	A	128	ILE
1	A	130	GLU
1	A	134	ARG
1	A	137	VAL
1	A	146	LYS
1	A	148	VAL
1	A	149	ARG
1	A	168	LYS
1	A	170	SER
1	A	183	GLN
1	A	187	VAL
1	A	199	MET
1	A	200	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	SER
1	A	210	ARG
1	A	214	ILE
1	A	220	THR
1	A	231	LYS
1	A	232	ASP
1	A	237	VAL
1	A	248	ARG
1	A	254	LYS
1	B	6	VAL
1	B	15	LEU
1	B	19	ILE
1	B	22	LEU
1	B	24	ASN
1	B	25	GLU
1	B	29	ASP
1	B	47	LEU
1	B	48	VAL
1	B	50	MET
1	B	53	ARG
1	B	64	ARG
1	B	65	ASN
1	B	70	LEU
1	B	88	LEU
1	B	95	ASP
1	B	102	THR
1	B	104	GLU
1	B	109	THR
1	B	115	GLN
1	B	116	LEU
1	B	118	LEU
1	B	119	LEU
1	B	131	MET
1	B	135	SER
1	B	136	THR
1	B	137	VAL
1	B	153	VAL
1	B	162	ILE
1	B	164	LYS
1	B	168	LYS
1	B	170	SER
1	B	188	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	190	ARG
1	B	198	THR
1	B	206	SER
1	B	217	LYS
1	B	227	LEU
1	B	231	LYS
1	B	232	ASP
1	B	237	VAL
1	B	248	ARG
1	B	256	ASP
1	C	1	MET
1	C	2	LEU
1	C	3	GLU
1	C	10	SER
1	C	19	ILE
1	C	22	LEU
1	C	42	SER
1	C	47	LEU
1	C	50	MET
1	C	53	ARG
1	C	57	PHE
1	C	62	CYS
1	C	64	ARG
1	C	65	ASN
1	C	70	LEU
1	C	89	SER
1	C	95	ASP
1	C	97	ASP
1	C	98	VAL
1	C	99	VAL
1	C	102	THR
1	C	107	GLU
1	C	108	LYS
1	C	109	THR
1	C	116	LEU
1	C	118	LEU
1	C	126	MET
1	C	128	ILE
1	C	131	MET
1	C	134	ARG
1	C	135	SER
1	C	136	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	137	VAL
1	C	148	VAL
1	C	153	VAL
1	C	159	THR
1	C	163	SER
1	C	170	SER
1	C	188	SER
1	C	190	ARG
1	C	196	GLU
1	C	198	THR
1	C	199	MET
1	C	201	GLU
1	C	206	SER
1	C	214	ILE
1	C	217	LYS
1	C	220	THR
1	C	227	LEU
1	C	233	SER
1	C	236	MET
1	C	237	VAL
1	C	243	ASN
1	C	248	ARG
1	D	2	LEU
1	D	3	GLU
1	D	7	GLN
1	D	10	SER
1	D	15	LEU
1	D	19	ILE
1	D	22	LEU
1	D	25	GLU
1	D	29	ASP
1	D	30	CYS
1	D	35	LEU
1	D	36	SER
1	D	38	GLN
1	D	42	SER
1	D	47	LEU
1	D	48	VAL
1	D	57	PHE
1	D	64	ARG
1	D	81	ILE
1	D	89	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	90	LEU
1	D	97	ASP
1	D	99	VAL
1	D	102	THR
1	D	119	LEU
1	D	121	ILE
1	D	125	SER
1	D	126	MET
1	D	133	TYR
1	D	134	ARG
1	D	137	VAL
1	D	143	GLU
1	D	162	ILE
1	D	163	SER
1	D	164	LYS
1	D	168	LYS
1	D	170	SER
1	D	177	GLN
1	D	189	ASP
1	D	190	ARG
1	D	195	VAL
1	D	198	THR
1	D	199	MET
1	D	201	GLU
1	D	202	PRO
1	D	217	LYS
1	D	228	LYS
1	D	231	LYS
1	D	232	ASP
1	D	243	ASN
1	E	1	MET
1	E	2	LEU
1	E	19	ILE
1	E	22	LEU
1	E	24	ASN
1	E	36	SER
1	E	42	SER
1	E	45	VAL
1	E	47	LEU
1	E	50	MET
1	E	51	LEU
1	E	53	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	64	ARG
1	E	70	LEU
1	E	80	LYS
1	E	94	ASP
1	E	99	VAL
1	E	100	THR
1	E	105	ASN
1	E	107	GLU
1	E	108	LYS
1	E	109	THR
1	E	117	LYS
1	E	119	LEU
1	E	121	ILE
1	E	128	ILE
1	E	130	GLU
1	E	132	ASP
1	E	136	THR
1	E	137	VAL
1	E	139	LEU
1	E	143	GLU
1	E	148	VAL
1	E	153	VAL
1	E	156	ASP
1	E	164	LYS
1	E	165	GLU
1	E	167	VAL
1	E	168	LYS
1	E	170	SER
1	E	188	SER
1	E	189	ASP
1	E	199	MET
1	E	203	ILE
1	E	217	LYS
1	E	220	THR
1	E	222	SER
1	E	237	VAL
1	E	241	ILE
1	E	243	ASN
1	E	248	ARG
1	E	251	LEU
1	F	2	LEU
1	F	6	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	7	GLN
1	F	19	ILE
1	F	22	LEU
1	F	30	CYS
1	F	45	VAL
1	F	47	LEU
1	F	50	MET
1	F	51	LEU
1	F	59	LYS
1	F	61	GLN
1	F	62	CYS
1	F	70	LEU
1	F	74	SER
1	F	76	SER
1	F	80	LYS
1	F	82	VAL
1	F	89	SER
1	F	91	ARG
1	F	93	ASP
1	F	94	ASP
1	F	97	ASP
1	F	98	VAL
1	F	99	VAL
1	F	100	THR
1	F	104	GLU
1	F	108	LYS
1	F	116	LEU
1	F	117	LYS
1	F	118	LEU
1	F	119	LEU
1	F	120	GLU
1	F	121	ILE
1	F	122	GLU
1	F	130	GLU
1	F	131	MET
1	F	132	ASP
1	F	135	SER
1	F	136	THR
1	F	137	VAL
1	F	148	VAL
1	F	156	ASP
1	F	164	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	165	GLU
1	F	167	VAL
1	F	168	LYS
1	F	170	SER
1	F	175	VAL
1	F	180	THR
1	F	187	VAL
1	F	190	ARG
1	F	198	THR
1	F	199	MET
1	F	200	GLU
1	F	214	ILE
1	F	217	LYS
1	F	231	LYS
1	F	232	ASP
1	F	233	SER
1	F	242	ASP
1	F	243	ASN
1	F	248	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	27	ASN
1	A	38	GLN
1	A	44	HIS
1	A	105	ASN
1	A	115	GLN
1	A	140	ASN
1	A	243	ASN
1	B	7	GLN
1	B	20	ASN
1	B	31	ASN
1	B	38	GLN
1	B	92	HIS
1	B	152	GLN
1	B	183	GLN
1	C	7	GLN
1	C	31	ASN
1	C	38	GLN
1	C	44	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	115	GLN
1	C	152	GLN
1	C	183	GLN
1	C	243	ASN
1	D	27	ASN
1	D	31	ASN
1	D	61	GLN
1	D	105	ASN
1	D	115	GLN
1	D	183	GLN
1	D	243	ASN
1	E	20	ASN
1	E	27	ASN
1	E	38	GLN
1	E	44	HIS
1	E	49	HIS
1	E	115	GLN
1	E	243	ASN
1	F	27	ASN
1	F	44	HIS
1	F	61	GLN
1	F	115	GLN
1	F	243	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	253/259 (97%)	-0.52	5 (1%) 65 45	57, 85, 159, 259	0
1	B	253/259 (97%)	-0.49	5 (1%) 65 45	57, 89, 164, 215	0
1	C	253/259 (97%)	-0.39	3 (1%) 76 58	60, 97, 165, 261	0
1	D	253/259 (97%)	-0.30	4 (1%) 70 51	68, 102, 166, 249	0
1	E	253/259 (97%)	-0.26	5 (1%) 65 45	69, 105, 178, 235	0
1	F	253/259 (97%)	-0.21	7 (2%) 55 35	67, 108, 169, 244	0
All	All	1518/1554 (97%)	-0.36	29 (1%) 66 46	57, 98, 169, 261	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	GLY	4.0
1	E	129	PRO	3.6
1	A	126	MET	3.2
1	C	126	MET	3.2
1	F	126	MET	3.2
1	F	131	MET	3.0
1	F	185	ALA	2.9
1	E	128	ILE	2.9
1	C	132	ASP	2.8
1	E	126	MET	2.8
1	A	123	ALA	2.7
1	F	128	ILE	2.6
1	B	126	MET	2.5
1	E	181	PHE	2.5
1	B	1	MET	2.3
1	F	132	ASP	2.3
1	A	187	VAL	2.2
1	B	131	MET	2.2
1	F	255	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	130	GLU	2.2
1	C	133	TYR	2.2
1	E	1	MET	2.2
1	D	132	ASP	2.2
1	D	131	MET	2.1
1	A	201	GLU	2.1
1	B	133	TYR	2.1
1	D	133	TYR	2.1
1	B	256	ASP	2.1
1	A	1	MET	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.