



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:06 AM UTC

PDB ID : 2HXY / pdb_00002hxy
Title : Crystal structure of human apo-eIF4AIII
Authors : Johansen, J.S.; Andersen, G.R.
Deposited on : 2006-08-04
Resolution : 3.30 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

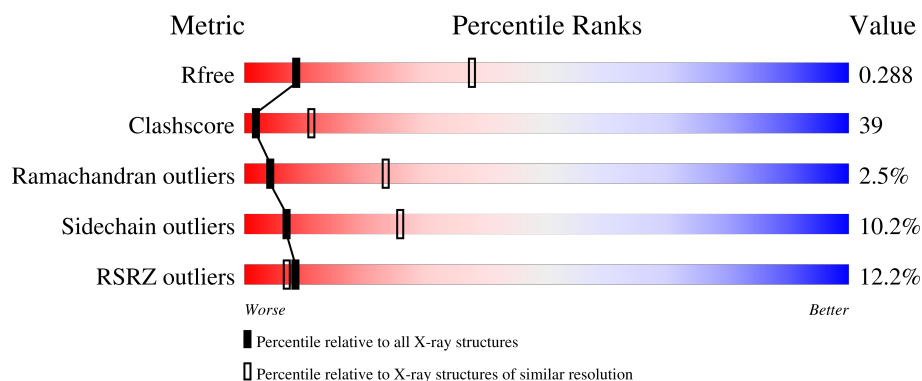
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	391	10% 40% 42% 13% ..
1	B	391	13% 39% 47% 10% ..
1	C	391	9% 38% 47% 11% ..
1	D	391	16% 37% 47% 11% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12080 atoms, of which 0 are hydrogens and 0 are deuteriums.

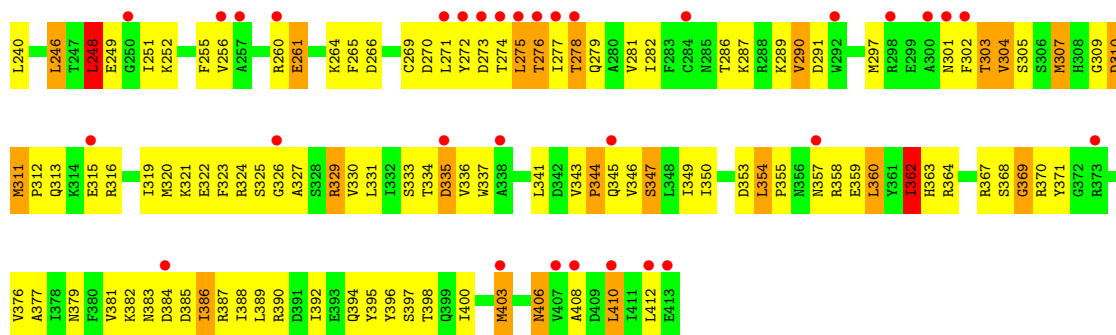
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable ATP-dependent RNA helicase DDX48.

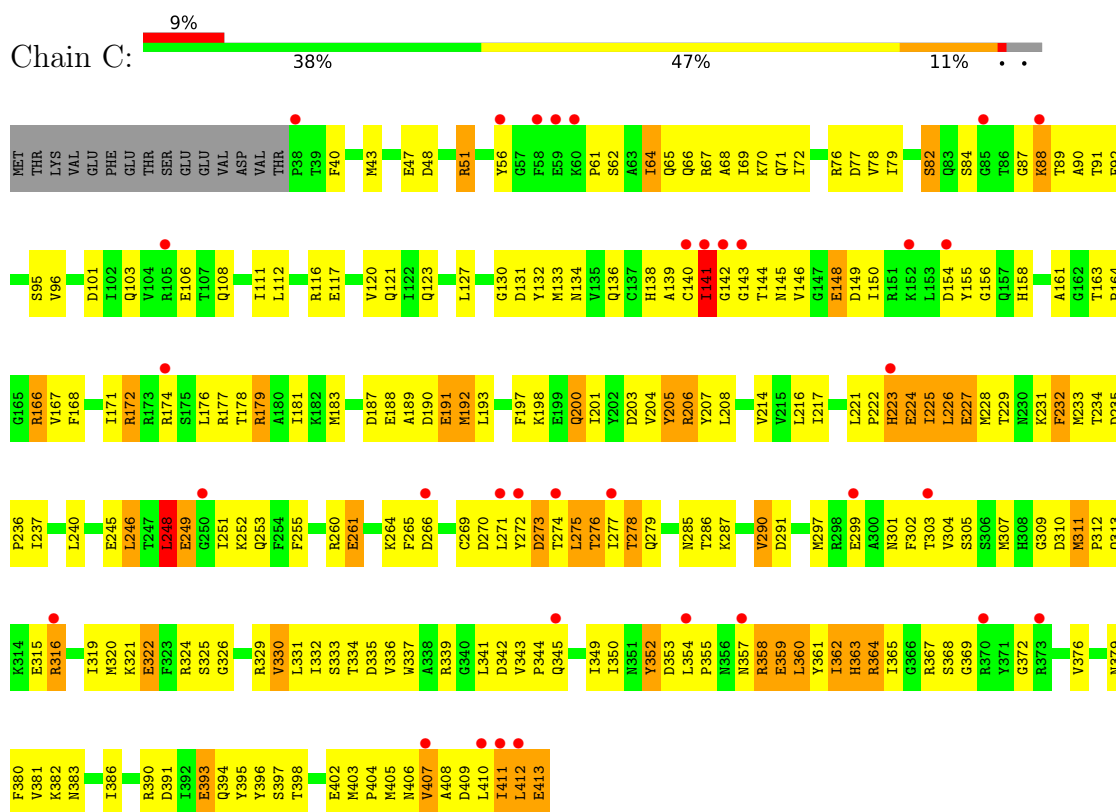
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			3020	1909	531	562	18			
1	B	376	Total	C	N	O	S	0	0	0
			3020	1909	531	562	18			
1	C	376	Total	C	N	O	S	0	0	0
			3020	1909	531	562	18			
1	D	376	Total	C	N	O	S	0	0	0
			3020	1909	531	562	18			

There are 8 discrepancies between the modelled and reference sequences:

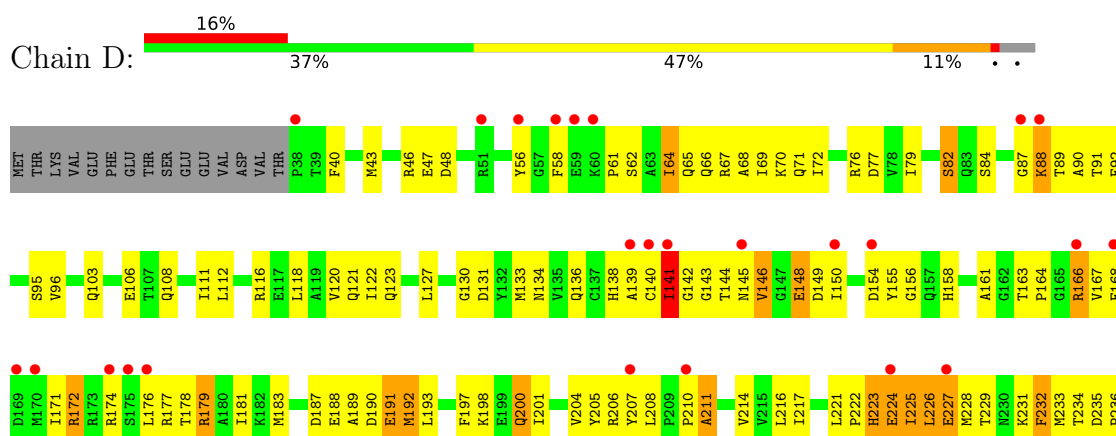
Chain	Residue	Modelled	Actual	Comment	Reference
A	412	LEU	-	cloning artifact	UNP P38919
A	413	GLU	-	cloning artifact	UNP P38919
B	412	LEU	-	cloning artifact	UNP P38919
B	413	GLU	-	cloning artifact	UNP P38919
C	412	LEU	-	cloning artifact	UNP P38919
C	413	GLU	-	cloning artifact	UNP P38919
D	412	LEU	-	cloning artifact	UNP P38919
D	413	GLU	-	cloning artifact	UNP P38919

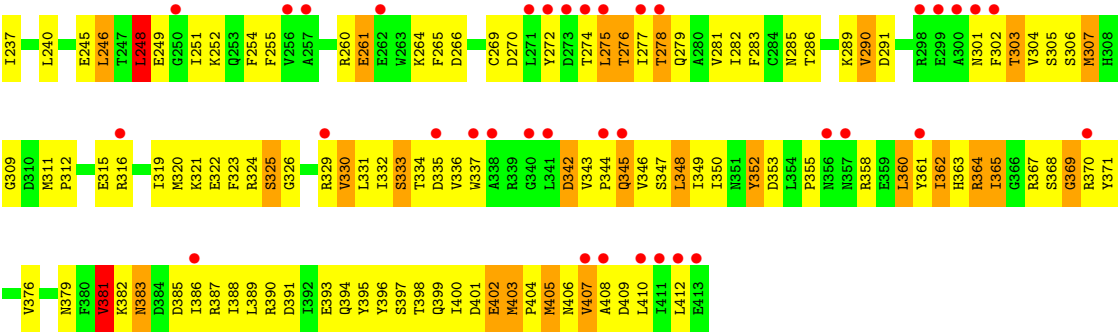


● Molecule 1: Probable ATP-dependent RNA helicase DDX48



● Molecule 1: Probable ATP-dependent RNA helicase DDX48





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.22Å 238.05Å 79.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 99.6 (50.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.308 0.262 , 0.288	Depositor DCC
R_{free} test set	1335 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12080	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	0/3068	1.27	41/4138 (1.0%)
1	B	0.71	1/3068 (0.0%)	1.20	26/4138 (0.6%)
1	C	0.68	0/3068	1.22	37/4138 (0.9%)
1	D	0.69	0/3068	1.23	35/4138 (0.8%)
All	All	0.70	1/12272 (0.0%)	1.23	139/16552 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	ILE	CA-CB	6.91	1.63	1.54

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	MET	CA-C-N	9.89	130.29	119.90
1	A	311	MET	C-N-CA	9.89	130.29	119.90
1	D	407	VAL	N-CA-C	-9.24	103.60	112.29
1	A	326	GLY	N-CA-C	-8.99	102.23	115.63
1	A	407	VAL	N-CA-C	-8.60	102.65	113.22
1	C	144	THR	N-CA-C	-8.55	102.74	113.01
1	A	144	THR	N-CA-C	-8.38	103.05	113.18
1	A	361	TYR	N-CA-C	-8.24	102.26	111.82
1	A	290	VAL	N-CA-C	-8.09	103.38	110.74
1	B	290	VAL	N-CA-C	-8.09	103.38	110.74
1	C	290	VAL	N-CA-C	-8.08	103.39	110.74
1	D	290	VAL	N-CA-C	-8.07	103.39	110.74
1	B	144	THR	N-CA-C	-8.06	103.34	113.01
1	D	221	LEU	CA-C-N	7.46	127.42	120.03
1	D	221	LEU	C-N-CA	7.46	127.42	120.03
1	B	221	LEU	CA-C-N	7.46	127.41	120.03
1	B	221	LEU	C-N-CA	7.46	127.41	120.03
1	C	221	LEU	CA-C-N	7.45	127.40	120.03
1	C	221	LEU	C-N-CA	7.45	127.40	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LEU	CA-C-N	7.43	127.39	120.03
1	A	221	LEU	C-N-CA	7.43	127.39	120.03
1	D	393	GLU	N-CA-C	-7.41	102.89	110.97
1	B	362	ILE	N-CA-C	-7.39	103.26	110.72
1	A	274	THR	CA-C-N	7.37	130.66	120.63
1	A	274	THR	C-N-CA	7.37	130.66	120.63
1	C	393	GLU	N-CA-C	-7.36	102.94	110.97
1	D	144	THR	N-CA-C	-7.20	104.46	113.18
1	D	304	VAL	N-CA-C	7.18	119.15	108.96
1	D	403	MET	N-CA-C	7.06	119.06	109.24
1	A	312	PRO	N-CA-C	7.05	121.44	110.80
1	C	309	GLY	N-CA-C	7.03	122.99	113.99
1	B	261	GLU	N-CA-C	6.98	119.78	111.33
1	A	261	GLU	N-CA-C	6.96	119.75	111.33
1	D	261	GLU	N-CA-C	6.95	119.73	111.33
1	C	261	GLU	N-CA-C	6.94	119.72	111.33
1	D	365	ILE	N-CA-C	6.90	119.66	112.83
1	D	88	LYS	N-CA-C	-6.81	105.09	113.19
1	D	333	SER	N-CA-C	6.77	118.48	108.60
1	C	88	LYS	N-CA-C	-6.73	105.06	113.20
1	C	352	TYR	N-CA-C	-6.67	104.04	111.71
1	A	356	ASN	N-CA-C	6.62	118.99	110.65
1	B	88	LYS	N-CA-C	-6.60	105.21	113.20
1	A	334	THR	N-CA-C	-6.53	100.80	110.46
1	B	359	GLU	N-CA-C	6.49	120.45	112.54
1	D	274	THR	N-CA-C	-6.45	104.02	112.41
1	C	225	ILE	N-CA-C	-6.39	102.88	111.44
1	A	225	ILE	N-CA-C	-6.36	102.91	111.44
1	D	225	ILE	N-CA-C	-6.36	102.92	111.44
1	B	225	ILE	N-CA-C	-6.35	102.93	111.44
1	C	412	LEU	N-CA-C	6.31	118.87	109.59
1	B	304	VAL	N-CA-C	6.22	117.79	108.96
1	B	226	LEU	N-CA-C	-6.21	104.60	111.36
1	C	71	GLN	N-CA-C	6.19	118.11	111.36
1	C	226	LEU	N-CA-C	-6.18	104.62	111.36
1	D	309	GLY	N-CA-C	6.18	121.34	113.24
1	A	226	LEU	N-CA-C	-6.18	104.62	111.36
1	B	71	GLN	N-CA-C	6.17	118.09	111.36
1	D	226	LEU	N-CA-C	-6.16	104.64	111.36
1	A	375	GLY	N-CA-C	6.14	121.03	111.08
1	D	307	MET	N-CA-C	6.13	118.10	108.96
1	B	403	MET	N-CA-C	6.11	120.26	109.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	MET	CA-C-N	6.08	127.00	120.13
1	C	311	MET	C-N-CA	6.08	127.00	120.13
1	D	71	GLN	N-CA-C	6.07	117.98	111.36
1	A	88	LYS	N-CA-C	-6.04	106.01	113.19
1	B	410	LEU	N-CA-C	-5.98	105.97	113.20
1	A	272	TYR	N-CA-C	5.93	118.50	111.33
1	A	359	GLU	N-CA-C	-5.92	103.72	113.50
1	A	405	MET	N-CA-C	-5.91	104.18	111.33
1	C	407	VAL	N-CA-C	-5.91	105.60	112.98
1	C	261	GLU	CB-CA-C	-5.85	100.74	110.68
1	D	261	GLU	CB-CA-C	-5.84	100.75	110.68
1	B	78	VAL	N-CA-C	5.84	116.89	108.48
1	B	261	GLU	CB-CA-C	-5.82	100.78	110.68
1	A	261	GLU	CB-CA-C	-5.82	100.79	110.68
1	C	205	TYR	N-CA-C	-5.82	105.07	111.82
1	A	56	TYR	N-CA-C	-5.80	105.46	112.54
1	C	409	ASP	N-CA-C	-5.80	106.20	113.28
1	C	333	SER	N-CA-C	5.80	117.88	109.07
1	B	148	GLU	N-CA-C	-5.77	105.13	111.82
1	D	56	TYR	N-CA-C	-5.72	105.56	112.54
1	A	410	LEU	N-CA-C	-5.72	106.53	112.93
1	C	403	MET	N-CA-C	5.68	122.36	109.81
1	A	315	GLU	N-CA-C	-5.68	106.49	113.41
1	C	56	TYR	N-CA-C	-5.67	105.62	112.54
1	C	148	GLU	N-CA-C	-5.66	105.26	111.82
1	C	304	VAL	N-CA-C	5.65	118.07	108.86
1	A	354	LEU	N-CA-C	-5.62	102.33	110.08
1	A	329	ARG	N-CA-C	5.61	118.59	111.69
1	A	409	ASP	N-CA-C	-5.60	106.11	113.17
1	C	286	THR	N-CA-C	5.59	118.34	109.50
1	A	286	THR	N-CA-C	5.55	118.28	109.50
1	B	286	THR	N-CA-C	5.54	118.25	109.50
1	B	155	TYR	N-CA-C	-5.53	105.63	112.38
1	D	286	THR	N-CA-C	5.53	118.23	109.50
1	C	155	TYR	N-CA-C	-5.53	105.64	112.38
1	D	408	ALA	N-CA-C	-5.48	107.16	112.97
1	D	155	TYR	N-CA-C	-5.47	105.71	112.38
1	C	47	GLU	N-CA-C	5.46	116.92	110.97
1	A	386	ILE	N-CA-C	-5.45	103.65	111.17
1	C	78	VAL	N-CA-C	5.44	117.23	108.85
1	B	248	LEU	N-CA-C	5.42	119.00	112.93
1	A	248	LEU	N-CA-C	5.39	118.97	112.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	248	LEU	N-CA-C	5.39	118.97	112.93
1	C	248	LEU	N-CA-C	5.39	118.97	112.93
1	B	237	ILE	CB-CA-C	-5.37	104.25	110.91
1	D	237	ILE	CB-CA-C	-5.36	104.26	110.91
1	B	212	THR	N-CA-C	5.36	118.09	110.10
1	C	237	ILE	CB-CA-C	-5.36	104.27	110.91
1	A	237	ILE	CB-CA-C	-5.35	104.28	110.91
1	A	78	VAL	N-CA-C	5.35	117.09	108.85
1	C	330	VAL	N-CA-C	5.35	115.41	108.35
1	C	311	MET	N-CA-C	5.32	118.37	110.39
1	D	304	VAL	CB-CA-C	-5.25	103.99	111.19
1	D	47	GLU	N-CA-C	5.24	116.68	110.97
1	B	311	MET	CA-C-N	5.23	125.64	119.99
1	B	311	MET	C-N-CA	5.23	125.64	119.99
1	C	273	ASP	CB-CA-C	-5.23	102.64	110.90
1	D	381	VAL	N-CA-C	5.22	115.58	107.28
1	A	59	GLU	N-CA-C	5.19	119.67	113.23
1	C	299	GLU	N-CA-C	-5.14	107.07	113.19
1	D	348	LEU	N-CA-C	5.14	116.69	107.80
1	A	155	TYR	N-CA-C	-5.14	106.11	112.38
1	C	245	GLU	N-CA-C	5.13	117.60	109.50
1	A	245	GLU	N-CA-C	5.12	117.60	109.50
1	A	71	GLN	N-CA-C	5.11	116.93	111.36
1	D	245	GLU	N-CA-C	5.10	117.56	109.50
1	D	306	SER	N-CA-C	5.09	117.69	109.40
1	A	148	GLU	N-CA-C	-5.08	105.83	111.36
1	B	304	VAL	CB-CA-C	-5.06	104.26	111.19
1	D	148	GLU	N-CA-C	-5.04	105.97	111.82
1	D	402	GLU	N-CA-C	-5.04	104.03	110.53
1	C	251	ILE	N-CA-C	5.03	115.55	108.36
1	A	251	ILE	N-CA-C	5.02	115.54	108.36
1	D	251	ILE	N-CA-C	5.02	115.54	108.36
1	A	388	ILE	CB-CA-C	-5.02	104.72	112.05
1	D	352	TYR	N-CA-C	-5.02	105.94	111.71
1	C	51	ARG	N-CA-C	-5.01	105.72	111.14
1	B	251	ILE	N-CA-C	5.01	115.53	108.36

There are no chirality outliers.

There are no planarity outliers.

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	3020	0	3075	236	0
1	B	3020	0	3075	226	1
1	C	3020	0	3075	243	0
1	D	3020	0	3075	257	0
All	All	12080	0	12300	953	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (953) 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:D:272:TYR:CD1	1:D:275:LEU:HD13	1.81	1.14
1:C:207:TYR:HA	1:D:210:PRO:HG3	1.32	1.10
1:A:312:PRO:HG2	1:A:315:GLU:HB3	1.30	1.09
1:D:276:THR:HG22	1:D:329:ARG:HB3	1.10	1.09
1:D:346:VAL:HG22	1:D:347:SER:H	1.18	1.09
1:C:116:ARG:HG2	1:C:141:ILE:HD13	1.38	1.05
1:D:116:ARG:HG2	1:D:141:ILE:HD13	1.37	1.04
1:B:116:ARG:HG2	1:B:141:ILE:HD13	1.38	1.04
1:B:383:ASN:O	1:B:386:ILE:HG22	1.61	1.00
1:A:116:ARG:HG2	1:A:141:ILE:HD13	1.39	1.00
1:D:222:PRO:HD2	1:D:225:ILE:HG13	1.44	0.99
1:B:222:PRO:HD2	1:B:225:ILE:HG13	1.44	0.98
1:A:222:PRO:HD2	1:A:225:ILE:HG13	1.44	0.98
1:D:272:TYR:HD1	1:D:275:LEU:HD13	1.14	0.97
1:C:222:PRO:HD2	1:C:225:ILE:HG13	1.44	0.95
1:D:276:THR:CG2	1:D:329:ARG:HB3	1.95	0.95
1:C:383:ASN:O	1:C:386:ILE:HG22	1.68	0.94
1:B:200:GLN:H	1:B:200:GLN:HE21	1.16	0.94
1:C:200:GLN:H	1:C:200:GLN:HE21	1.15	0.93
1:A:355:PRO:HB2	1:A:360:LEU:HD11	1.51	0.93
1:D:276:THR:HG22	1:D:329:ARG:CB	1.97	0.92
1:D:200:GLN:H	1:D:200:GLN:HE21	1.16	0.92
1:C:200:GLN:O	1:C:204:VAL:HG23	1.72	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLN:H	1:A:200:GLN:HE21	1.16	0.90
1:B:200:GLN:O	1:B:204:VAL:HG23	1.72	0.89
1:D:200:GLN:O	1:D:204:VAL:HG23	1.72	0.89
1:A:290:VAL:HG13	1:A:332:ILE:HG22	1.53	0.89
1:A:200:GLN:O	1:A:204:VAL:HG23	1.72	0.88
1:A:275:LEU:HD21	1:A:330:VAL:CG2	2.05	0.86
1:C:246:LEU:CD1	1:C:341:LEU:HG	2.05	0.86
1:B:320:MET:HE2	1:B:320:MET:HA	1.57	0.85
1:D:355:PRO:CB	1:D:360:LEU:HD11	2.05	0.85
1:D:235:ASP:OD2	1:D:344:PRO:HA	1.77	0.85
1:D:252:LYS:HB2	1:D:376:VAL:HG22	1.59	0.84
1:A:307:MET:HE3	1:A:320:MET:HE3	1.59	0.83
1:C:290:VAL:HG13	1:C:332:ILE:HG22	1.57	0.83
1:A:410:LEU:HD23	1:A:410:LEU:O	1.78	0.83
1:D:320:MET:HA	1:D:320:MET:HE2	1.61	0.82
1:A:112:LEU:HB2	1:A:192:MET:HE1	1.62	0.82
1:C:200:GLN:H	1:C:200:GLN:NE2	1.78	0.81
1:A:320:MET:HE1	1:A:331:LEU:CD2	2.10	0.81
1:B:200:GLN:H	1:B:200:GLN:NE2	1.78	0.80
1:C:112:LEU:HB2	1:C:192:MET:HE1	1.60	0.80
1:C:246:LEU:HD13	1:C:341:LEU:HG	1.63	0.80
1:D:200:GLN:H	1:D:200:GLN:NE2	1.79	0.80
1:A:200:GLN:H	1:A:200:GLN:NE2	1.79	0.79
1:B:381:VAL:HG11	1:B:389:LEU:HD22	1.64	0.79
1:D:272:TYR:HA	1:D:275:LEU:HB2	1.65	0.79
1:D:112:LEU:HB2	1:D:192:MET:HE1	1.64	0.79
1:D:346:VAL:HG22	1:D:347:SER:N	1.98	0.79
1:A:320:MET:HE1	1:A:331:LEU:HD22	1.63	0.78
1:B:112:LEU:HB2	1:B:192:MET:HE1	1.64	0.78
1:D:334:THR:OG1	1:D:336:VAL:HG13	1.84	0.78
1:D:272:TYR:HA	1:D:275:LEU:CB	2.14	0.77
1:A:355:PRO:CB	1:A:360:LEU:HD11	2.15	0.77
1:B:367:ARG:NH1	1:B:369:GLY:HA2	1.99	0.77
1:C:362:ILE:HB	1:C:396:TYR:CE2	2.20	0.76
1:C:341:LEU:HD12	1:C:341:LEU:H	1.51	0.76
1:A:341:LEU:HD12	1:A:341:LEU:H	1.50	0.76
1:A:277:ILE:HG21	1:A:410:LEU:HD22	1.67	0.76
1:A:317:GLU:O	1:A:321:LYS:HG3	1.85	0.76
1:A:383:ASN:O	1:A:386:ILE:HG22	1.86	0.76
1:C:189:ALA:HA	1:C:192:MET:HG3	1.67	0.76
1:A:116:ARG:CG	1:A:141:ILE:HD13	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:CG	1:B:141:ILE:HD13	2.17	0.75
1:C:312:PRO:O	1:C:316:ARG:HG2	1.87	0.75
1:A:123:GLN:HE21	1:A:138:HIS:HA	1.51	0.74
1:B:276:THR:HG22	1:B:329:ARG:HB3	1.69	0.74
1:C:123:GLN:NE2	1:C:138:HIS:HA	2.03	0.74
1:D:116:ARG:CG	1:D:141:ILE:HD13	2.17	0.74
1:D:285:ASN:HD21	1:D:355:PRO:HA	1.51	0.74
1:A:123:GLN:NE2	1:A:138:HIS:HA	2.03	0.74
1:B:62:SER:HB3	1:B:65:GLN:HG3	1.68	0.74
1:C:360:LEU:HD12	1:C:360:LEU:C	2.12	0.73
1:C:123:GLN:HE21	1:C:138:HIS:HA	1.52	0.73
1:A:200:GLN:HE21	1:A:200:GLN:N	1.87	0.73
1:C:200:GLN:HE21	1:C:200:GLN:N	1.87	0.73
1:C:181:ILE:HG21	1:C:208:LEU:HD22	1.69	0.73
1:C:62:SER:HB3	1:C:65:GLN:HG3	1.70	0.72
1:B:304:VAL:HG12	1:B:330:VAL:HB	1.71	0.72
1:A:62:SER:HB3	1:A:65:GLN:HG3	1.71	0.72
1:A:312:PRO:CG	1:A:315:GLU:HB3	2.16	0.72
1:B:62:SER:HB3	1:B:65:GLN:CG	2.19	0.72
1:D:355:PRO:HB3	1:D:360:LEU:HD11	1.69	0.72
1:C:276:THR:HG22	1:C:329:ARG:HB3	1.71	0.72
1:A:287:LYS:HD3	1:A:310:ASP:OD2	1.90	0.72
1:D:62:SER:HB3	1:D:65:GLN:HG3	1.70	0.72
1:C:62:SER:HB3	1:C:65:GLN:CG	2.19	0.72
1:A:189:ALA:HA	1:A:192:MET:HG3	1.70	0.72
1:B:123:GLN:HE21	1:B:138:HIS:HA	1.55	0.72
1:A:322:GLU:O	1:A:325:SER:HB3	1.89	0.72
1:B:116:ARG:HG2	1:B:141:ILE:HG21	1.72	0.71
1:D:360:LEU:C	1:D:360:LEU:HD12	2.15	0.71
1:D:189:ALA:HA	1:D:192:MET:HG3	1.72	0.71
1:D:123:GLN:HE21	1:D:138:HIS:HA	1.56	0.71
1:D:200:GLN:HE21	1:D:200:GLN:N	1.87	0.71
1:D:311:MET:HE2	1:D:315:GLU:CD	2.15	0.71
1:D:316:ARG:HH11	1:D:316:ARG:HG3	1.55	0.71
1:C:261:GLU:HG2	1:C:382:LYS:HZ2	1.55	0.71
1:D:255:PHE:CE1	1:D:402:GLU:HG3	2.26	0.71
1:A:275:LEU:HD21	1:A:330:VAL:HG22	1.72	0.71
1:C:214:VAL:O	1:C:233:MET:HE2	1.91	0.71
1:C:337:TRP:CZ2	1:C:344:PRO:HD3	2.26	0.71
1:C:116:ARG:CG	1:C:141:ILE:HD13	2.18	0.70
1:B:189:ALA:HA	1:B:192:MET:HG3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLU:O	1:B:319:ILE:HG12	1.90	0.70
1:D:141:ILE:HA	1:D:166:ARG:HD2	1.72	0.70
1:A:214:VAL:O	1:A:233:MET:HE2	1.91	0.70
1:B:269:CYS:O	1:B:272:TYR:HB3	1.91	0.70
1:B:272:TYR:CE1	1:B:302:PHE:HD1	2.10	0.70
1:D:123:GLN:NE2	1:D:138:HIS:HA	2.06	0.70
1:B:200:GLN:HE21	1:B:200:GLN:N	1.87	0.70
1:B:297:MET:O	1:B:302:PHE:HD2	1.74	0.70
1:C:276:THR:HG22	1:C:329:ARG:CB	2.22	0.70
1:A:362:ILE:HB	1:A:396:TYR:CE2	2.27	0.70
1:B:214:VAL:O	1:B:233:MET:HE2	1.91	0.70
1:B:246:LEU:HB3	1:B:362:ILE:CD1	2.22	0.70
1:A:360:LEU:C	1:A:360:LEU:HD12	2.17	0.70
1:D:214:VAL:O	1:D:233:MET:HE2	1.91	0.70
1:B:123:GLN:NE2	1:B:138:HIS:HA	2.07	0.69
1:A:358:ARG:O	1:A:358:ARG:HG2	1.91	0.69
1:D:410:LEU:HD23	1:D:410:LEU:O	1.93	0.69
1:A:272:TYR:CD1	1:A:275:LEU:HD13	2.27	0.69
1:D:311:MET:HB2	1:D:316:ARG:HD2	1.75	0.69
1:A:311:MET:HB3	1:A:312:PRO:HD2	1.75	0.68
1:D:303:THR:HG23	1:D:329:ARG:HB2	1.75	0.68
1:C:275:LEU:C	1:C:275:LEU:HD23	2.17	0.68
1:C:311:MET:HE2	1:C:315:GLU:OE1	1.93	0.68
1:C:413:GLU:CB	1:D:174:ARG:HH22	2.06	0.68
1:D:62:SER:HB3	1:D:65:GLN:CG	2.23	0.68
1:D:281:VAL:HB	1:D:349:ILE:HD13	1.74	0.68
1:D:346:VAL:CG2	1:D:347:SER:H	2.03	0.68
1:A:275:LEU:C	1:A:275:LEU:HD23	2.18	0.67
1:A:181:ILE:HG21	1:A:208:LEU:HD22	1.77	0.67
1:A:228:MET:HG2	1:A:232:PHE:CE2	2.29	0.67
1:A:62:SER:HB3	1:A:65:GLN:CG	2.24	0.67
1:D:228:MET:HG2	1:D:232:PHE:CE2	2.29	0.67
1:C:274:THR:HG21	1:C:407:VAL:HG21	1.77	0.67
1:B:228:MET:HG2	1:B:232:PHE:CE2	2.29	0.67
1:D:355:PRO:HB2	1:D:360:LEU:HD11	1.76	0.67
1:A:248:LEU:H	1:A:248:LEU:HD12	1.60	0.67
1:C:228:MET:HG2	1:C:232:PHE:CE2	2.29	0.66
1:C:315:GLU:O	1:C:319:ILE:HG12	1.95	0.66
1:A:143:GLY:HA2	1:A:146:VAL:HG13	1.78	0.66
1:C:279:GLN:HA	1:C:329:ARG:O	1.96	0.66
1:D:272:TYR:O	1:D:275:LEU:HB3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LEU:HD12	1:C:248:LEU:H	1.60	0.66
1:C:255:PHE:CE1	1:C:402:GLU:HG3	2.30	0.66
1:C:402:GLU:O	1:C:404:PRO:HD3	1.94	0.66
1:A:140:CYS:O	1:A:141:ILE:HB	1.93	0.66
1:C:331:LEU:HD12	1:C:332:ILE:N	2.10	0.66
1:B:255:PHE:HA	1:B:379:ASN:O	1.96	0.66
1:D:141:ILE:HG23	1:D:142:GLY:N	2.11	0.66
1:D:143:GLY:HA2	1:D:146:VAL:HG13	1.78	0.66
1:A:141:ILE:HG23	1:A:142:GLY:N	2.11	0.66
1:B:272:TYR:O	1:B:275:LEU:HB3	1.94	0.66
1:B:248:LEU:HD12	1:B:248:LEU:H	1.61	0.66
1:C:285:ASN:HD21	1:C:355:PRO:HA	1.60	0.66
1:D:370:ARG:HG2	1:D:371:TYR:CE1	2.31	0.66
1:B:141:ILE:HG23	1:B:142:GLY:N	2.10	0.66
1:D:140:CYS:O	1:D:141:ILE:HB	1.95	0.65
1:C:320:MET:HE2	1:C:320:MET:HA	1.77	0.65
1:C:141:ILE:HG23	1:C:142:GLY:N	2.12	0.65
1:C:272:TYR:CZ	1:C:302:PHE:HD1	2.13	0.65
1:A:339:ARG:HD2	1:A:342:ASP:OD2	1.96	0.65
1:C:166:ARG:HB2	1:C:166:ARG:HH11	1.60	0.65
1:B:410:LEU:HD23	1:B:410:LEU:O	1.97	0.65
1:A:141:ILE:HA	1:A:166:ARG:HD2	1.78	0.65
1:D:248:LEU:H	1:D:248:LEU:HD12	1.61	0.65
1:B:276:THR:HG22	1:B:329:ARG:CB	2.26	0.65
1:B:181:ILE:HG21	1:B:208:LEU:HD22	1.78	0.65
1:C:140:CYS:O	1:C:141:ILE:HB	1.97	0.65
1:C:216:LEU:HD23	1:C:216:LEU:C	2.23	0.64
1:A:272:TYR:HD1	1:A:275:LEU:HD13	1.61	0.64
1:B:172:ARG:O	1:B:174:ARG:HD3	1.98	0.64
1:C:203:ASP:O	1:C:206:ARG:CB	2.45	0.64
1:D:167:VAL:O	1:D:171:ILE:HG13	1.97	0.64
1:D:181:ILE:HG21	1:D:208:LEU:HD22	1.78	0.64
1:A:216:LEU:HD23	1:A:216:LEU:C	2.23	0.64
1:B:205:TYR:HA	1:B:208:LEU:HD12	1.80	0.64
1:D:412:LEU:HD12	1:D:412:LEU:O	1.98	0.64
1:B:316:ARG:HG3	1:B:316:ARG:HH11	1.61	0.64
1:C:368:SER:HB3	1:C:372:GLY:N	2.12	0.64
1:B:167:VAL:O	1:B:171:ILE:HG13	1.97	0.64
1:C:261:GLU:HG2	1:C:382:LYS:NZ	2.13	0.64
1:A:274:THR:O	1:A:277:ILE:HB	1.98	0.64
1:B:222:PRO:HD2	1:B:225:ILE:CG1	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:TYR:HA	1:D:210:PRO:CG	2.21	0.64
1:B:319:ILE:O	1:B:322:GLU:HB2	1.98	0.64
1:D:216:LEU:C	1:D:216:LEU:HD23	2.23	0.63
1:A:172:ARG:O	1:A:174:ARG:HD3	1.98	0.63
1:C:77:ASP:HB3	1:C:233:MET:CG	2.28	0.63
1:C:172:ARG:O	1:C:174:ARG:HD3	1.98	0.63
1:B:163:THR:O	1:B:167:VAL:HG23	1.98	0.63
1:C:275:LEU:HD23	1:C:276:THR:N	2.13	0.63
1:B:272:TYR:CE1	1:B:302:PHE:CD1	2.87	0.63
1:D:82:SER:HA	1:D:88:LYS:HE2	1.81	0.63
1:A:77:ASP:HB3	1:A:233:MET:CG	2.29	0.63
1:A:320:MET:HA	1:A:320:MET:HE2	1.81	0.63
1:B:82:SER:HA	1:B:88:LYS:HE2	1.81	0.63
1:B:143:GLY:HA2	1:B:146:VAL:HG13	1.80	0.63
1:A:116:ARG:HG2	1:A:141:ILE:HG21	1.81	0.63
1:B:141:ILE:HA	1:B:166:ARG:HD2	1.79	0.63
1:D:43:MET:HE3	1:D:66:GLN:HG3	1.80	0.63
1:D:163:THR:O	1:D:167:VAL:HG23	1.99	0.63
1:B:216:LEU:C	1:B:216:LEU:HD23	2.23	0.63
1:C:307:MET:HE3	1:C:319:ILE:HB	1.79	0.63
1:C:141:ILE:HA	1:C:166:ARG:HD2	1.81	0.62
1:A:275:LEU:HD23	1:A:276:THR:N	2.14	0.62
1:B:166:ARG:HH11	1:B:166:ARG:HB2	1.64	0.62
1:C:167:VAL:O	1:C:171:ILE:HG13	1.98	0.62
1:C:312:PRO:HG2	1:C:315:GLU:HB3	1.82	0.62
1:D:77:ASP:HB3	1:D:233:MET:CG	2.30	0.62
1:D:275:LEU:C	1:D:275:LEU:HD23	2.25	0.62
1:D:275:LEU:HD21	1:D:330:VAL:CG2	2.29	0.62
1:B:43:MET:HE3	1:B:66:GLN:HG3	1.81	0.62
1:C:319:ILE:O	1:C:322:GLU:HB2	1.99	0.62
1:A:167:VAL:O	1:A:171:ILE:HG13	1.99	0.62
1:B:275:LEU:C	1:B:275:LEU:HD23	2.25	0.62
1:C:362:ILE:HG23	1:C:363:HIS:N	2.14	0.62
1:A:283:PHE:CE1	1:A:364:ARG:HG2	2.35	0.62
1:D:172:ARG:O	1:D:174:ARG:HD3	1.99	0.62
1:C:274:THR:HA	1:C:277:ILE:HG13	1.80	0.62
1:C:205:TYR:HA	1:C:208:LEU:HD12	1.82	0.61
1:A:82:SER:HA	1:A:88:LYS:HE2	1.81	0.61
1:C:316:ARG:HG3	1:C:316:ARG:HH11	1.63	0.61
1:B:276:THR:HG22	1:B:329:ARG:CG	2.30	0.61
1:C:166:ARG:HB2	1:C:166:ARG:NH1	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:LEU:HB3	1:C:362:ILE:CD1	2.29	0.61
1:C:290:VAL:HG13	1:C:332:ILE:CG2	2.28	0.61
1:A:412:LEU:HD12	1:A:412:LEU:O	2.01	0.61
1:B:141:ILE:CG2	1:B:142:GLY:N	2.63	0.61
1:C:143:GLY:HA2	1:C:146:VAL:HG13	1.81	0.61
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.66	0.61
1:D:116:ARG:HG3	1:D:116:ARG:HH11	1.66	0.61
1:C:163:THR:O	1:C:167:VAL:HG23	1.99	0.61
1:C:64:ILE:HG13	1:C:65:GLN:N	2.16	0.61
1:B:210:PRO:O	1:B:211:ALA:HB3	2.00	0.61
1:D:279:GLN:HG2	1:D:329:ARG:NH2	2.16	0.61
1:D:246:LEU:HB3	1:D:362:ILE:CD1	2.31	0.60
1:A:279:GLN:HA	1:A:329:ARG:O	2.01	0.60
1:A:346:VAL:HG22	1:A:348:LEU:H	1.67	0.60
1:C:82:SER:HA	1:C:88:LYS:HE2	1.81	0.60
1:B:141:ILE:HG23	1:B:142:GLY:H	1.67	0.60
1:A:43:MET:HE3	1:A:66:GLN:HG3	1.83	0.60
1:C:362:ILE:CG2	1:C:363:HIS:N	2.64	0.60
1:D:391:ASP:O	1:D:395:TYR:HB2	2.01	0.60
1:A:303:THR:HG23	1:A:303:THR:O	2.01	0.60
1:B:164:PRO:HB2	1:B:197:PHE:HD2	1.66	0.60
1:C:360:LEU:HD12	1:C:361:TYR:N	2.16	0.60
1:C:43:MET:HE3	1:C:66:GLN:HG3	1.82	0.60
1:A:64:ILE:HG13	1:A:65:GLN:N	2.16	0.60
1:A:222:PRO:HD2	1:A:225:ILE:CG1	2.26	0.59
1:B:355:PRO:HB3	1:B:360:LEU:HD11	1.84	0.59
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.68	0.59
1:D:222:PRO:HD2	1:D:225:ILE:CG1	2.26	0.59
1:B:64:ILE:HG13	1:B:65:GLN:N	2.17	0.59
1:B:77:ASP:HB3	1:B:233:MET:CG	2.31	0.59
1:B:96:VAL:HA	1:B:183:MET:HE1	1.85	0.59
1:B:367:ARG:CZ	1:B:369:GLY:HA2	2.32	0.59
1:C:354:LEU:HD21	1:C:379:ASN:HB3	1.84	0.59
1:D:367:ARG:NH1	1:D:369:GLY:HA2	2.17	0.59
1:A:246:LEU:HA	1:A:367:ARG:O	2.03	0.59
1:A:166:ARG:HH11	1:A:166:ARG:HB2	1.67	0.59
1:B:116:ARG:HG2	1:B:141:ILE:CD1	2.25	0.59
1:D:166:ARG:HB2	1:D:166:ARG:HH11	1.68	0.59
1:D:336:VAL:HG23	1:D:336:VAL:O	2.03	0.59
1:A:116:ARG:HG3	1:A:116:ARG:HH11	1.68	0.59
1:D:381:VAL:O	1:D:381:VAL:HG23	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLN:HB3	1:B:323:PHE:CE1	2.38	0.58
1:B:362:ILE:HB	1:B:396:TYR:CE2	2.38	0.58
1:A:67:ARG:HG3	1:A:67:ARG:HH11	1.68	0.58
1:C:246:LEU:HB3	1:C:362:ILE:HD11	1.84	0.58
1:C:311:MET:HB3	1:C:312:PRO:HD2	1.85	0.58
1:D:116:ARG:HG2	1:D:141:ILE:HG21	1.85	0.58
1:D:255:PHE:HA	1:D:379:ASN:O	2.03	0.58
1:A:68:ALA:O	1:A:72:ILE:HG13	2.04	0.58
1:D:362:ILE:HD13	1:D:362:ILE:O	2.04	0.58
1:D:272:TYR:HA	1:D:275:LEU:HB3	1.86	0.58
1:B:320:MET:HE1	1:B:331:LEU:HD22	1.85	0.58
1:C:357:ASN:C	1:C:359:GLU:H	2.11	0.58
1:C:362:ILE:HB	1:C:396:TYR:CZ	2.39	0.58
1:C:77:ASP:HB3	1:C:233:MET:HG2	1.86	0.58
1:B:140:CYS:O	1:B:141:ILE:HB	2.04	0.57
1:B:289:LYS:HD3	1:B:353:ASP:OD1	2.02	0.57
1:A:320:MET:HE1	1:A:331:LEU:HD21	1.86	0.57
1:A:360:LEU:C	1:A:360:LEU:CD1	2.77	0.57
1:B:360:LEU:C	1:B:360:LEU:HD12	2.29	0.57
1:D:283:PHE:CE1	1:D:364:ARG:HG3	2.39	0.57
1:B:412:LEU:O	1:B:412:LEU:HD12	2.04	0.57
1:C:320:MET:O	1:C:321:LYS:C	2.47	0.57
1:A:277:ILE:HG22	1:A:278:THR:HG22	1.86	0.57
1:A:348:LEU:HD22	1:A:410:LEU:HD11	1.87	0.57
1:B:388:ILE:O	1:B:392:ILE:HG13	2.03	0.57
1:D:141:ILE:CG2	1:D:142:GLY:N	2.67	0.57
1:A:282:ILE:HG12	1:A:350:ILE:HB	1.85	0.57
1:C:116:ARG:HG2	1:C:141:ILE:HG21	1.85	0.57
1:C:255:PHE:HA	1:C:379:ASN:O	2.04	0.57
1:D:275:LEU:HD23	1:D:276:THR:N	2.19	0.57
1:A:406:ASN:HB3	1:A:409:ASP:OD2	2.05	0.57
1:B:275:LEU:HD23	1:B:276:THR:N	2.19	0.57
1:D:311:MET:HB2	1:D:316:ARG:CD	2.35	0.57
1:B:166:ARG:HB2	1:B:166:ARG:NH1	2.19	0.57
1:A:254:PHE:HA	1:A:401:ASP:O	2.05	0.57
1:A:255:PHE:HA	1:A:379:ASN:O	2.04	0.57
1:B:309:GLY:C	1:B:311:MET:H	2.13	0.57
1:A:274:THR:O	1:A:274:THR:HG22	2.03	0.57
1:B:390:ARG:O	1:B:394:GLN:HG2	2.05	0.57
1:B:255:PHE:HD2	1:B:400:ILE:HG22	1.69	0.56
1:D:246:LEU:HB3	1:D:362:ILE:HD11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HB3	1:B:362:ILE:HD13	1.87	0.56
1:B:334:THR:O	1:B:336:VAL:N	2.39	0.56
1:B:358:ARG:HD2	1:B:395:TYR:CD1	2.40	0.56
1:D:334:THR:O	1:D:336:VAL:N	2.38	0.56
1:D:316:ARG:HG3	1:D:316:ARG:NH1	2.21	0.56
1:D:349:ILE:HG21	1:D:365:ILE:HG22	1.87	0.56
1:A:297:MET:O	1:A:302:PHE:HB2	2.05	0.56
1:B:305:SER:O	1:B:331:LEU:HD12	2.04	0.56
1:A:272:TYR:HE1	1:A:330:VAL:HG21	1.70	0.56
1:B:362:ILE:CG2	1:B:363:HIS:N	2.69	0.56
1:D:282:ILE:HG12	1:D:350:ILE:HB	1.88	0.56
1:A:355:PRO:HB2	1:A:360:LEU:CD1	2.33	0.56
1:B:281:VAL:HB	1:B:349:ILE:HD13	1.86	0.56
1:C:275:LEU:HD21	1:C:330:VAL:HG22	1.87	0.56
1:C:412:LEU:HD12	1:C:412:LEU:O	2.05	0.56
1:B:304:VAL:HG12	1:B:330:VAL:CB	2.35	0.56
1:D:164:PRO:HB2	1:D:197:PHE:HD2	1.71	0.56
1:C:355:PRO:HB3	1:C:360:LEU:HD11	1.87	0.56
1:D:166:ARG:HB2	1:D:166:ARG:NH1	2.21	0.56
1:A:246:LEU:HD13	1:A:341:LEU:HG	1.88	0.55
1:A:276:THR:C	1:A:278:THR:N	2.63	0.55
1:B:346:VAL:HG22	1:B:347:SER:H	1.70	0.55
1:C:96:VAL:HA	1:C:183:MET:HE1	1.87	0.55
1:C:272:TYR:CZ	1:C:302:PHE:CD1	2.93	0.55
1:D:381:VAL:HG11	1:D:389:LEU:HD22	1.87	0.55
1:C:222:PRO:HD2	1:C:225:ILE:CG1	2.26	0.55
1:C:391:ASP:O	1:C:395:TYR:HB2	2.05	0.55
1:C:408:ALA:O	1:C:411:ILE:HG13	2.06	0.55
1:D:64:ILE:HG13	1:D:65:GLN:N	2.21	0.55
1:A:96:VAL:HA	1:A:183:MET:HE1	1.88	0.55
1:D:223:HIS:ND1	1:D:223:HIS:N	2.53	0.55
1:D:272:TYR:HD1	1:D:275:LEU:CD1	2.03	0.55
1:A:276:THR:HG22	1:A:329:ARG:HB3	1.88	0.55
1:B:96:VAL:HA	1:B:183:MET:CE	2.37	0.55
1:D:312:PRO:O	1:D:316:ARG:HG2	2.07	0.55
1:A:362:ILE:HD13	1:A:362:ILE:O	2.07	0.55
1:C:207:TYR:CA	1:D:210:PRO:HG3	2.22	0.55
1:B:193:LEU:HD21	1:B:228:MET:HE1	1.89	0.55
1:A:141:ILE:CG2	1:A:142:GLY:N	2.70	0.55
1:C:187:ASP:OD1	1:C:188:GLU:HG3	2.07	0.55
1:B:385:ASP:C	1:B:387:ARG:N	2.62	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PHE:CZ	1:B:61:PRO:HB3	2.42	0.54
1:C:178:THR:O	1:C:179:ARG:C	2.50	0.54
1:A:356:ASN:O	1:A:357:ASN:HB3	2.07	0.54
1:B:287:LYS:HD3	1:B:310:ASP:OD2	2.08	0.54
1:C:141:ILE:CG2	1:C:142:GLY:N	2.71	0.54
1:B:223:HIS:ND1	1:B:223:HIS:N	2.54	0.54
1:A:77:ASP:HB3	1:A:233:MET:HG2	1.88	0.54
1:C:164:PRO:HB2	1:C:197:PHE:HD2	1.72	0.54
1:D:276:THR:C	1:D:278:THR:N	2.63	0.54
1:A:187:ASP:OD1	1:A:188:GLU:HG3	2.07	0.54
1:D:96:VAL:HA	1:D:183:MET:HE1	1.90	0.54
1:D:345:GLN:O	1:D:345:GLN:HG3	2.08	0.54
1:A:275:LEU:CD2	1:A:276:THR:N	2.71	0.54
1:A:360:LEU:HA	1:A:363:HIS:HB3	1.89	0.54
1:B:111:ILE:O	1:B:161:ALA:HA	2.08	0.54
1:B:368:SER:O	1:B:370:ARG:N	2.39	0.54
1:D:367:ARG:CZ	1:D:369:GLY:HA2	2.37	0.54
1:D:123:GLN:HG2	1:D:127:LEU:HD12	1.89	0.54
1:C:276:THR:C	1:C:278:THR:N	2.63	0.53
1:B:168:PHE:HE1	1:B:207:TYR:CE2	2.26	0.53
1:C:331:LEU:HD12	1:C:332:ILE:H	1.73	0.53
1:D:187:ASP:OD1	1:D:188:GLU:HG3	2.09	0.53
1:A:189:ALA:O	1:A:190:ASP:C	2.51	0.53
1:B:406:ASN:C	1:B:408:ALA:H	2.16	0.53
1:D:168:PHE:HE1	1:D:207:TYR:CE2	2.27	0.53
1:C:96:VAL:HA	1:C:183:MET:CE	2.39	0.53
1:C:275:LEU:CD2	1:C:276:THR:N	2.71	0.53
1:D:92:PHE:O	1:D:95:SER:HB2	2.08	0.53
1:A:96:VAL:HA	1:A:183:MET:CE	2.39	0.53
1:A:163:THR:O	1:A:167:VAL:HG23	2.08	0.53
1:B:326:GLY:O	1:B:327:ALA:C	2.52	0.53
1:B:360:LEU:HA	1:B:363:HIS:HB3	1.90	0.53
1:A:123:GLN:HG2	1:A:127:LEU:HD12	1.91	0.53
1:B:146:VAL:HA	1:B:149:ASP:HB2	1.91	0.53
1:D:290:VAL:HG13	1:D:332:ILE:HG22	1.91	0.53
1:A:272:TYR:CE2	1:A:302:PHE:HD1	2.27	0.53
1:B:133:MET:O	1:B:134:ASN:C	2.52	0.53
1:B:297:MET:HE2	1:B:302:PHE:CG	2.44	0.53
1:D:405:MET:SD	1:D:405:MET:N	2.82	0.53
1:A:349:ILE:O	1:A:377:ALA:HA	2.08	0.52
1:C:313:GLN:HA	1:C:316:ARG:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ASN:C	1:C:359:GLU:N	2.66	0.52
1:D:255:PHE:HD2	1:D:400:ILE:HG22	1.74	0.52
1:D:396:TYR:O	1:D:397:SER:HB2	2.08	0.52
1:C:77:ASP:OD2	1:C:233:MET:HA	2.08	0.52
1:C:249:GLU:O	1:C:367:ARG:HD3	2.10	0.52
1:D:329:ARG:O	1:D:330:VAL:HG23	2.10	0.52
1:D:395:TYR:HD2	1:D:396:TYR:CE1	2.27	0.52
1:A:166:ARG:HB2	1:A:166:ARG:NH1	2.24	0.52
1:A:178:THR:O	1:A:179:ARG:C	2.51	0.52
1:A:283:PHE:CD1	1:A:364:ARG:HG2	2.45	0.52
1:C:311:MET:HE2	1:C:315:GLU:CD	2.34	0.52
1:C:367:ARG:NH1	1:C:369:GLY:HA2	2.24	0.52
1:A:276:THR:HG22	1:A:329:ARG:CB	2.40	0.52
1:B:346:VAL:HG22	1:B:347:SER:N	2.24	0.52
1:A:341:LEU:H	1:A:341:LEU:CD1	2.22	0.52
1:B:123:GLN:HG2	1:B:127:LEU:HD12	1.90	0.52
1:B:349:ILE:O	1:B:377:ALA:HA	2.09	0.52
1:C:223:HIS:ND1	1:C:223:HIS:N	2.53	0.52
1:C:352:TYR:HA	1:C:380:PHE:CD2	2.45	0.52
1:C:413:GLU:HB3	1:D:174:ARG:HH22	1.73	0.52
1:A:193:LEU:HD21	1:A:228:MET:HE1	1.92	0.52
1:D:96:VAL:HA	1:D:183:MET:CE	2.39	0.52
1:D:315:GLU:O	1:D:319:ILE:HG12	2.08	0.52
1:B:341:LEU:HD12	1:B:341:LEU:H	1.74	0.52
1:C:275:LEU:HD21	1:C:330:VAL:CG2	2.38	0.52
1:D:337:TRP:CD1	1:D:342:ASP:O	2.63	0.52
1:C:316:ARG:HG3	1:C:316:ARG:NH1	2.25	0.52
1:D:285:ASN:OD1	1:D:353:ASP:HB3	2.10	0.52
1:A:168:PHE:HE1	1:A:207:TYR:CE2	2.27	0.52
1:A:174:ARG:HG2	1:A:174:ARG:HH11	1.74	0.52
1:A:272:TYR:O	1:A:275:LEU:HB3	2.10	0.52
1:D:77:ASP:HB3	1:D:233:MET:HG2	1.91	0.52
1:C:123:GLN:HG2	1:C:127:LEU:HD12	1.93	0.51
1:A:77:ASP:OD2	1:A:233:MET:HA	2.10	0.51
1:B:316:ARG:HG3	1:B:316:ARG:NH1	2.25	0.51
1:D:360:LEU:C	1:D:360:LEU:CD1	2.83	0.51
1:A:76:ARG:HG3	1:A:76:ARG:HH11	1.74	0.51
1:A:140:CYS:O	1:A:141:ILE:CB	2.59	0.51
1:A:320:MET:O	1:A:324:ARG:HG3	2.09	0.51
1:C:336:VAL:HG13	1:C:337:TRP:N	2.25	0.51
1:D:146:VAL:HA	1:D:149:ASP:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:O	1:C:161:ALA:HA	2.11	0.51
1:C:272:TYR:O	1:C:275:LEU:HB3	2.10	0.51
1:B:320:MET:HE1	1:B:331:LEU:CD2	2.40	0.51
1:D:193:LEU:HD21	1:D:228:MET:HE1	1.93	0.51
1:C:413:GLU:HA	1:D:174:ARG:NH2	2.25	0.51
1:A:40:PHE:CZ	1:A:61:PRO:HB3	2.45	0.51
1:C:112:LEU:CB	1:C:192:MET:HE1	2.37	0.51
1:D:77:ASP:OD2	1:D:233:MET:HA	2.11	0.51
1:D:178:THR:O	1:D:179:ARG:C	2.54	0.51
1:B:312:PRO:O	1:B:316:ARG:HG2	2.11	0.51
1:A:285:ASN:OD1	1:A:353:ASP:CB	2.59	0.51
1:B:48:ASP:OD2	1:B:133:MET:HG2	2.10	0.51
1:B:77:ASP:HB3	1:B:233:MET:HG2	1.93	0.51
1:C:246:LEU:HD11	1:C:341:LEU:HG	1.92	0.51
1:C:255:PHE:CZ	1:C:402:GLU:HG3	2.46	0.51
1:D:76:ARG:HG3	1:D:76:ARG:HH11	1.76	0.51
1:D:320:MET:HB3	1:D:324:ARG:NH1	2.26	0.51
1:A:223:HIS:ND1	1:A:223:HIS:N	2.54	0.51
1:A:261:GLU:OE2	1:A:264:LYS:HD2	2.11	0.51
1:D:197:PHE:O	1:D:198:LYS:C	2.54	0.51
1:D:261:GLU:OE2	1:D:264:LYS:HD2	2.11	0.51
1:D:362:ILE:CG2	1:D:363:HIS:N	2.74	0.51
1:A:146:VAL:HA	1:A:149:ASP:HB2	1.93	0.50
1:A:205:TYR:HA	1:A:208:LEU:HD12	1.93	0.50
1:D:272:TYR:CD1	1:D:275:LEU:CD1	2.75	0.50
1:B:320:MET:O	1:B:321:LYS:C	2.55	0.50
1:B:362:ILE:HG23	1:B:363:HIS:N	2.25	0.50
1:C:146:VAL:HA	1:C:149:ASP:HB2	1.92	0.50
1:C:261:GLU:OE2	1:C:264:LYS:HD2	2.11	0.50
1:C:272:TYR:CE2	1:C:302:PHE:HD1	2.29	0.50
1:A:111:ILE:O	1:A:161:ALA:HA	2.11	0.50
1:C:92:PHE:O	1:C:95:SER:HB2	2.12	0.50
1:C:322:GLU:O	1:C:325:SER:HB3	2.11	0.50
1:B:276:THR:C	1:B:278:THR:N	2.63	0.50
1:C:76:ARG:HH11	1:C:76:ARG:HG3	1.76	0.50
1:D:275:LEU:C	1:D:277:ILE:N	2.70	0.50
1:A:164:PRO:HB2	1:A:197:PHE:HD2	1.76	0.50
1:B:246:LEU:HD13	1:B:341:LEU:HG	1.94	0.50
1:D:140:CYS:O	1:D:141:ILE:CB	2.59	0.50
1:A:275:LEU:CD2	1:A:330:VAL:CG2	2.86	0.50
1:B:256:VAL:HG22	1:B:403:MET:SD	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLY:O	1:B:311:MET:N	2.44	0.50
1:C:360:LEU:O	1:C:361:TYR:C	2.53	0.50
1:C:40:PHE:CZ	1:C:61:PRO:HB3	2.47	0.50
1:D:321:LYS:O	1:D:325:SER:HB3	2.12	0.50
1:D:387:ARG:O	1:D:390:ARG:N	2.39	0.50
1:B:261:GLU:OE2	1:B:264:LYS:HD2	2.11	0.50
1:D:362:ILE:HB	1:D:396:TYR:CE2	2.46	0.50
1:B:234:THR:O	1:B:235:ASP:C	2.55	0.49
1:B:362:ILE:C	1:B:364:ARG:N	2.68	0.49
1:C:203:ASP:O	1:C:206:ARG:HB2	2.10	0.49
1:C:355:PRO:CB	1:C:360:LEU:HD11	2.41	0.49
1:D:48:ASP:OD2	1:D:133:MET:HG2	2.12	0.49
1:D:234:THR:O	1:D:235:ASP:C	2.55	0.49
1:D:320:MET:O	1:D:324:ARG:N	2.40	0.49
1:A:92:PHE:O	1:A:95:SER:HB2	2.11	0.49
1:A:190:ASP:HA	1:A:225:ILE:HD11	1.94	0.49
1:A:272:TYR:CE1	1:A:330:VAL:HG21	2.47	0.49
1:A:320:MET:O	1:A:321:LYS:C	2.53	0.49
1:D:76:ARG:HG3	1:D:76:ARG:NH1	2.27	0.49
1:D:164:PRO:HD2	1:D:197:PHE:CD2	2.46	0.49
1:A:285:ASN:OD1	1:A:353:ASP:HB2	2.12	0.49
1:C:206:ARG:NH1	1:D:206:ARG:HD2	2.27	0.49
1:C:272:TYR:CE2	1:C:302:PHE:CD1	3.00	0.49
1:A:133:MET:O	1:A:134:ASN:C	2.55	0.49
1:B:164:PRO:HD2	1:B:197:PHE:CD2	2.47	0.49
1:B:189:ALA:O	1:B:190:ASP:C	2.55	0.49
1:D:133:MET:O	1:D:134:ASN:C	2.56	0.49
1:B:178:THR:O	1:B:179:ARG:C	2.55	0.49
1:D:333:SER:OG	1:D:334:THR:N	2.45	0.49
1:A:290:VAL:HG13	1:A:332:ILE:CG2	2.34	0.49
1:A:385:ASP:C	1:A:387:ARG:N	2.62	0.49
1:B:140:CYS:O	1:B:141:ILE:CB	2.61	0.49
1:B:181:ILE:HG21	1:B:208:LEU:CD2	2.42	0.49
1:B:275:LEU:C	1:B:277:ILE:N	2.70	0.49
1:A:388:ILE:O	1:A:392:ILE:HG13	2.12	0.49
1:C:92:PHE:CD1	1:C:92:PHE:C	2.90	0.49
1:D:275:LEU:CD2	1:D:276:THR:N	2.76	0.49
1:A:76:ARG:HG3	1:A:76:ARG:NH1	2.28	0.49
1:C:363:HIS:ND1	1:C:363:HIS:C	2.70	0.49
1:A:234:THR:O	1:A:235:ASP:C	2.55	0.49
1:A:381:VAL:HG23	1:A:381:VAL:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:TYR:O	1:B:397:SER:C	2.53	0.49
1:C:278:THR:OG1	1:C:279:GLN:N	2.46	0.49
1:A:40:PHE:CE1	1:A:61:PRO:HB3	2.48	0.49
1:A:197:PHE:O	1:A:201:ILE:HG12	2.13	0.49
1:C:394:GLN:HE21	1:C:394:GLN:HA	1.78	0.49
1:A:376:VAL:HG12	1:A:377:ALA:N	2.28	0.48
1:B:164:PRO:HB2	1:B:197:PHE:CD2	2.47	0.48
1:C:234:THR:O	1:C:235:ASP:C	2.55	0.48
1:C:274:THR:HA	1:C:277:ILE:CD1	2.44	0.48
1:D:205:TYR:HA	1:D:208:LEU:HD12	1.94	0.48
1:D:278:THR:OG1	1:D:279:GLN:N	2.46	0.48
1:A:278:THR:OG1	1:A:279:GLN:N	2.46	0.48
1:A:312:PRO:C	1:A:314:LYS:H	2.21	0.48
1:A:407:VAL:C	1:A:409:ASP:H	2.21	0.48
1:C:193:LEU:HD13	1:C:224:GLU:OE2	2.13	0.48
1:B:40:PHE:CE1	1:B:61:PRO:HB3	2.48	0.48
1:C:381:VAL:HG23	1:C:381:VAL:O	2.12	0.48
1:D:111:ILE:O	1:D:161:ALA:HA	2.13	0.48
1:D:320:MET:HE2	1:D:320:MET:CA	2.37	0.48
1:D:404:PRO:O	1:D:406:ASN:N	2.46	0.48
1:A:279:GLN:CA	1:A:329:ARG:O	2.62	0.48
1:B:228:MET:HG2	1:B:232:PHE:CZ	2.49	0.48
1:B:278:THR:OG1	1:B:279:GLN:N	2.46	0.48
1:A:228:MET:HG2	1:A:232:PHE:CZ	2.49	0.48
1:A:277:ILE:HG21	1:A:410:LEU:CD2	2.39	0.48
1:C:274:THR:HA	1:C:277:ILE:CG1	2.44	0.48
1:D:368:SER:O	1:D:370:ARG:N	2.46	0.48
1:C:154:ASP:C	1:C:156:GLY:N	2.71	0.48
1:C:413:GLU:CG	1:D:174:ARG:HH22	2.26	0.48
1:C:197:PHE:O	1:C:198:LYS:C	2.57	0.48
1:D:190:ASP:HA	1:D:225:ILE:HD11	1.96	0.48
1:D:323:PHE:O	1:D:324:ARG:C	2.56	0.48
1:D:228:MET:HG2	1:D:232:PHE:CZ	2.49	0.48
1:B:146:VAL:O	1:B:150:ILE:HG13	2.14	0.48
1:B:252:LYS:HB2	1:B:376:VAL:HG22	1.95	0.48
1:B:275:LEU:CD2	1:B:276:THR:N	2.76	0.48
1:C:67:ARG:HG3	1:C:67:ARG:HH11	1.79	0.48
1:C:172:ARG:C	1:C:174:ARG:H	2.22	0.48
1:C:205:TYR:CZ	1:C:232:PHE:HB2	2.49	0.48
1:D:40:PHE:CZ	1:D:61:PRO:HB3	2.49	0.48
1:D:118:LEU:O	1:D:122:ILE:HG13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ARG:C	1:D:174:ARG:H	2.22	0.48
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.79	0.48
1:B:343:VAL:HG23	1:B:345:GLN:HE21	1.79	0.48
1:D:146:VAL:O	1:D:150:ILE:HG13	2.14	0.48
1:C:228:MET:HG2	1:C:232:PHE:CZ	2.49	0.47
1:D:279:GLN:CG	1:D:329:ARG:NH2	2.76	0.47
1:A:246:LEU:CD1	1:A:341:LEU:HG	2.44	0.47
1:C:48:ASP:OD2	1:C:133:MET:HG2	2.14	0.47
1:C:261:GLU:CD	1:C:382:LYS:HZ3	2.20	0.47
1:C:357:ASN:O	1:C:359:GLU:N	2.48	0.47
1:A:235:ASP:OD2	1:A:345:GLN:HG3	2.14	0.47
1:B:154:ASP:C	1:B:156:GLY:N	2.71	0.47
1:B:177:ARG:HG3	1:B:177:ARG:HH11	1.80	0.47
1:C:76:ARG:HG3	1:C:76:ARG:NH1	2.28	0.47
1:C:140:CYS:O	1:C:141:ILE:CB	2.61	0.47
1:D:205:TYR:CG	1:D:232:PHE:HD1	2.32	0.47
1:B:76:ARG:HG3	1:B:76:ARG:HH11	1.79	0.47
1:B:205:TYR:CZ	1:B:232:PHE:HB2	2.49	0.47
1:B:337:TRP:CZ2	1:B:344:PRO:HD3	2.50	0.47
1:C:360:LEU:O	1:C:363:HIS:N	2.47	0.47
1:A:275:LEU:C	1:A:277:ILE:N	2.70	0.47
1:A:297:MET:O	1:A:302:PHE:HD2	1.97	0.47
1:A:383:ASN:O	1:A:386:ILE:CG2	2.60	0.47
1:B:187:ASP:OD1	1:B:188:GLU:HG3	2.14	0.47
1:D:210:PRO:O	1:D:211:ALA:HB3	2.14	0.47
1:C:261:GLU:CG	1:C:382:LYS:NZ	2.77	0.47
1:C:275:LEU:C	1:C:275:LEU:CD2	2.87	0.47
1:D:77:ASP:HB3	1:D:233:MET:HG3	1.95	0.47
1:D:276:THR:O	1:D:329:ARG:NH1	2.48	0.47
1:A:146:VAL:O	1:A:150:ILE:HG13	2.15	0.47
1:A:197:PHE:O	1:A:198:LYS:C	2.57	0.47
1:A:205:TYR:CZ	1:A:232:PHE:HB2	2.49	0.47
1:C:193:LEU:HD21	1:C:228:MET:HE1	1.95	0.47
1:D:319:ILE:O	1:D:322:GLU:HB2	2.14	0.47
1:D:388:ILE:O	1:D:391:ASP:N	2.47	0.47
1:A:275:LEU:C	1:A:277:ILE:H	2.23	0.47
1:A:315:GLU:O	1:A:319:ILE:HG12	2.15	0.47
1:A:385:ASP:O	1:A:386:ILE:C	2.58	0.47
1:B:77:ASP:OD2	1:B:233:MET:HA	2.14	0.47
1:B:190:ASP:HA	1:B:225:ILE:HD11	1.95	0.47
1:C:77:ASP:HB3	1:C:233:MET:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ASP:HA	1:C:225:ILE:HD11	1.97	0.47
1:C:275:LEU:C	1:C:277:ILE:N	2.69	0.47
1:D:189:ALA:O	1:D:190:ASP:C	2.55	0.47
1:D:205:TYR:CZ	1:D:232:PHE:HB2	2.49	0.47
1:A:92:PHE:CD1	1:A:92:PHE:C	2.93	0.47
1:A:341:LEU:HD12	1:A:341:LEU:N	2.26	0.47
1:B:92:PHE:CD1	1:B:92:PHE:C	2.92	0.47
1:B:385:ASP:C	1:B:387:ARG:H	2.23	0.47
1:C:133:MET:O	1:C:134:ASN:C	2.56	0.47
1:C:390:ARG:HA	1:C:390:ARG:HD2	1.54	0.47
1:B:164:PRO:HD2	1:B:197:PHE:CE2	2.50	0.47
1:B:271:LEU:O	1:B:272:TYR:C	2.57	0.47
1:B:370:ARG:HG2	1:B:371:TYR:CE1	2.50	0.47
1:A:193:LEU:HD13	1:A:224:GLU:OE2	2.15	0.46
1:A:222:PRO:C	1:A:224:GLU:H	2.23	0.46
1:C:168:PHE:HE1	1:C:207:TYR:CE2	2.33	0.46
1:C:222:PRO:C	1:C:224:GLU:H	2.23	0.46
1:D:272:TYR:CZ	1:D:302:PHE:HD1	2.33	0.46
1:D:272:TYR:CA	1:D:275:LEU:HB3	2.45	0.46
1:A:227:GLU:O	1:A:231:LYS:HB2	2.16	0.46
1:B:197:PHE:O	1:B:201:ILE:HG12	2.14	0.46
1:B:275:LEU:HD21	1:B:330:VAL:CG2	2.45	0.46
1:B:382:LYS:O	1:B:383:ASN:C	2.58	0.46
1:B:77:ASP:HB3	1:B:233:MET:HG3	1.97	0.46
1:C:336:VAL:HG13	1:C:337:TRP:H	1.80	0.46
1:D:171:ILE:HG12	1:D:176:LEU:HD23	1.98	0.46
1:C:68:ALA:O	1:C:72:ILE:HG13	2.16	0.46
1:C:139:ALA:HA	1:C:161:ALA:O	2.15	0.46
1:C:269:CYS:O	1:C:272:TYR:HB3	2.16	0.46
1:D:367:ARG:NH2	1:D:369:GLY:HA2	2.31	0.46
1:D:382:LYS:O	1:D:383:ASN:C	2.58	0.46
1:B:205:TYR:CG	1:B:232:PHE:HD1	2.32	0.46
1:B:222:PRO:C	1:B:224:GLU:H	2.23	0.46
1:B:355:PRO:CB	1:B:360:LEU:HD11	2.45	0.46
1:C:227:GLU:O	1:C:231:LYS:HB2	2.16	0.46
1:C:248:LEU:HD12	1:C:248:LEU:N	2.29	0.46
1:D:46:ARG:NE	1:D:133:MET:HE3	2.30	0.46
1:D:272:TYR:C	1:D:275:LEU:HB3	2.39	0.46
1:A:313:GLN:HG3	1:A:313:GLN:O	2.15	0.46
1:B:92:PHE:O	1:B:95:SER:HB2	2.15	0.46
1:B:116:ARG:CG	1:B:141:ILE:HG21	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:THR:C	1:C:277:ILE:HG13	2.41	0.46
1:D:399:GLN:NE2	1:D:401:ASP:OD1	2.44	0.46
1:C:349:ILE:HG22	1:C:350:ILE:N	2.30	0.46
1:D:197:PHE:O	1:D:201:ILE:HG12	2.15	0.46
1:D:275:LEU:C	1:D:277:ILE:H	2.23	0.46
1:A:79:ILE:HD13	1:A:229:THR:HG21	1.98	0.46
1:A:145:ASN:OD1	1:A:148:GLU:HB3	2.16	0.46
1:A:337:TRP:CD1	1:A:342:ASP:O	2.68	0.46
1:B:76:ARG:HG3	1:B:76:ARG:NH1	2.31	0.46
1:B:357:ASN:O	1:B:358:ARG:C	2.59	0.46
1:C:177:ARG:HG3	1:C:177:ARG:HH11	1.80	0.46
1:D:227:GLU:O	1:D:231:LYS:HB2	2.16	0.46
1:A:205:TYR:CG	1:A:232:PHE:HD1	2.32	0.46
1:C:334:THR:O	1:C:336:VAL:N	2.49	0.46
1:C:339:ARG:HB2	1:C:342:ASP:OD2	2.16	0.46
1:C:341:LEU:H	1:C:341:LEU:CD1	2.26	0.46
1:D:136:GLN:O	1:D:158:HIS:HB2	2.16	0.46
1:D:154:ASP:C	1:D:156:GLY:N	2.71	0.46
1:A:112:LEU:CB	1:A:192:MET:HE1	2.39	0.45
1:A:275:LEU:C	1:A:275:LEU:CD2	2.87	0.45
1:B:172:ARG:C	1:B:174:ARG:H	2.22	0.45
1:B:275:LEU:C	1:B:277:ILE:H	2.23	0.45
1:D:345:GLN:O	1:D:345:GLN:CG	2.64	0.45
1:A:272:TYR:HA	1:A:275:LEU:HB3	1.97	0.45
1:B:307:MET:HG3	1:B:333:SER:HB2	1.97	0.45
1:C:189:ALA:O	1:C:190:ASP:C	2.59	0.45
1:C:275:LEU:C	1:C:277:ILE:H	2.23	0.45
1:C:307:MET:CE	1:C:319:ILE:HB	2.44	0.45
1:D:68:ALA:O	1:D:72:ILE:HG13	2.15	0.45
1:A:48:ASP:OD1	1:A:48:ASP:N	2.50	0.45
1:C:79:ILE:HD13	1:C:229:THR:HG21	1.98	0.45
1:D:87:GLY:C	1:D:89:THR:H	2.24	0.45
1:D:174:ARG:HH11	1:D:174:ARG:HG2	1.81	0.45
1:D:248:LEU:HD12	1:D:248:LEU:N	2.29	0.45
1:B:227:GLU:O	1:B:231:LYS:HB2	2.16	0.45
1:C:164:PRO:HD2	1:C:197:PHE:CD2	2.52	0.45
1:D:69:ILE:O	1:D:70:LYS:C	2.59	0.45
1:D:92:PHE:CD1	1:D:92:PHE:C	2.94	0.45
1:D:106:GLU:O	1:D:108:GLN:HG3	2.17	0.45
1:A:311:MET:CB	1:A:312:PRO:HD2	2.43	0.45
1:A:355:PRO:CB	1:A:360:LEU:CD1	2.91	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PHE:O	1:B:198:LYS:C	2.58	0.45
1:B:301:ASN:HD22	1:B:301:ASN:C	2.23	0.45
1:C:146:VAL:O	1:C:150:ILE:HG13	2.16	0.45
1:C:285:ASN:OD1	1:C:353:ASP:HB2	2.15	0.45
1:D:222:PRO:C	1:D:224:GLU:H	2.23	0.45
1:A:77:ASP:HB3	1:A:233:MET:HG3	1.96	0.45
1:A:248:LEU:HD12	1:A:248:LEU:N	2.29	0.45
1:B:90:ALA:O	1:B:91:THR:C	2.59	0.45
1:B:248:LEU:HD12	1:B:248:LEU:N	2.29	0.45
1:D:48:ASP:OD1	1:D:48:ASP:N	2.49	0.45
1:D:79:ILE:HD13	1:D:229:THR:HG21	1.99	0.45
1:D:210:PRO:O	1:D:211:ALA:CB	2.65	0.45
1:A:67:ARG:O	1:A:68:ALA:C	2.60	0.45
1:A:90:ALA:O	1:A:91:THR:C	2.57	0.45
1:D:40:PHE:CE1	1:D:61:PRO:HB3	2.51	0.45
1:D:325:SER:OG	1:D:326:GLY:N	2.49	0.45
1:D:346:VAL:HG13	1:D:348:LEU:H	1.80	0.45
1:A:358:ARG:O	1:A:395:TYR:CE2	2.70	0.45
1:B:191:GLU:OE1	1:B:191:GLU:HA	2.16	0.45
1:C:90:ALA:O	1:C:91:THR:C	2.59	0.45
1:C:205:TYR:CG	1:C:232:PHE:HD1	2.34	0.45
1:D:164:PRO:HD2	1:D:197:PHE:CE2	2.51	0.45
1:D:193:LEU:HD13	1:D:224:GLU:OE2	2.17	0.45
1:B:106:GLU:O	1:B:108:GLN:HG3	2.17	0.45
1:B:136:GLN:O	1:B:158:HIS:HB2	2.17	0.45
1:C:154:ASP:OD1	1:D:329:ARG:HG3	2.17	0.45
1:C:360:LEU:C	1:C:360:LEU:CD1	2.84	0.45
1:A:367:ARG:NH2	1:A:369:GLY:O	2.51	0.44
1:A:405:MET:O	1:A:407:VAL:HG13	2.17	0.44
1:B:130:GLY:O	1:B:131:ASP:C	2.60	0.44
1:C:130:GLY:O	1:C:131:ASP:C	2.60	0.44
1:C:393:GLU:HG2	1:C:398:THR:O	2.17	0.44
1:A:76:ARG:CZ	1:A:324:ARG:NH2	2.80	0.44
1:A:191:GLU:OE1	1:A:191:GLU:HA	2.17	0.44
1:A:320:MET:HE2	1:A:320:MET:CA	2.46	0.44
1:B:118:LEU:O	1:B:122:ILE:HG13	2.17	0.44
1:C:174:ARG:HG2	1:C:174:ARG:HH11	1.81	0.44
1:A:315:GLU:O	1:A:318:SER:HB3	2.18	0.44
1:B:46:ARG:NE	1:B:133:MET:HE3	2.31	0.44
1:A:323:PHE:CD2	1:A:323:PHE:C	2.95	0.44
1:B:187:ASP:HA	1:B:217:ILE:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:VAL:O	1:B:291:ASP:C	2.61	0.44
1:D:145:ASN:OD1	1:D:148:GLU:HB3	2.17	0.44
1:D:360:LEU:O	1:D:363:HIS:HB3	2.17	0.44
1:D:381:VAL:O	1:D:381:VAL:CG2	2.64	0.44
1:B:67:ARG:HG3	1:B:67:ARG:HH11	1.82	0.44
1:B:112:LEU:CB	1:B:192:MET:HE1	2.41	0.44
1:A:354:LEU:CG	1:A:381:VAL:HG12	2.47	0.44
1:B:281:VAL:HB	1:B:349:ILE:CD1	2.48	0.44
1:C:40:PHE:CE1	1:C:61:PRO:HB3	2.53	0.44
1:C:120:VAL:O	1:C:121:GLN:C	2.60	0.44
1:D:276:THR:O	1:D:277:ILE:C	2.61	0.44
1:B:193:LEU:HD13	1:B:224:GLU:OE2	2.18	0.44
1:B:385:ASP:O	1:B:386:ILE:C	2.61	0.44
1:C:43:MET:CE	1:C:66:GLN:HG3	2.48	0.44
1:C:171:ILE:HG12	1:C:176:LEU:HD23	2.00	0.44
1:D:177:ARG:HG3	1:D:177:ARG:HH11	1.81	0.44
1:A:293:LEU:HG	1:A:332:ILE:HD13	2.00	0.44
1:B:48:ASP:OD1	1:B:48:ASP:N	2.51	0.44
1:B:303:THR:HG23	1:B:329:ARG:HB2	2.00	0.44
1:A:336:VAL:HG13	1:A:337:TRP:N	2.33	0.44
1:B:120:VAL:O	1:B:121:GLN:C	2.60	0.44
1:C:276:THR:O	1:C:277:ILE:C	2.60	0.44
1:A:116:ARG:CG	1:A:141:ILE:HG21	2.47	0.43
1:B:68:ALA:O	1:B:72:ILE:HG13	2.17	0.43
1:A:48:ASP:OD2	1:A:133:MET:HG2	2.18	0.43
1:A:269:CYS:O	1:A:270:ASP:C	2.62	0.43
1:A:344:PRO:C	1:A:346:VAL:H	2.26	0.43
1:A:354:LEU:HG	1:A:381:VAL:HG12	2.00	0.43
1:C:191:GLU:HA	1:C:191:GLU:OE1	2.18	0.43
1:A:276:THR:O	1:A:277:ILE:C	2.60	0.43
1:A:290:VAL:O	1:A:291:ASP:C	2.61	0.43
1:B:145:ASN:OD1	1:B:148:GLU:HB3	2.18	0.43
1:D:228:MET:CG	1:D:232:PHE:CZ	3.02	0.43
1:A:164:PRO:HD2	1:A:197:PHE:CD2	2.53	0.43
1:C:297:MET:O	1:C:302:PHE:HD2	2.01	0.43
1:D:265:PHE:O	1:D:266:ASP:C	2.61	0.43
1:A:120:VAL:O	1:A:123:GLN:HB3	2.19	0.43
1:B:51:ARG:HD3	1:B:132:TYR:CD2	2.54	0.43
1:C:320:MET:HB3	1:C:324:ARG:NH1	2.33	0.43
1:D:130:GLY:O	1:D:131:ASP:C	2.61	0.43
1:D:164:PRO:HB2	1:D:197:PHE:CD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:MET:CG	1:A:232:PHE:CZ	3.02	0.43
1:B:228:MET:CG	1:B:232:PHE:CZ	3.02	0.43
1:C:265:PHE:O	1:C:266:ASP:C	2.61	0.43
1:D:43:MET:CE	1:D:66:GLN:HG3	2.45	0.43
1:D:269:CYS:O	1:D:270:ASP:C	2.62	0.43
1:A:120:VAL:O	1:A:121:GLN:C	2.61	0.43
1:A:233:MET:HG2	1:A:236:PRO:HB3	2.01	0.43
1:B:272:TYR:C	1:B:272:TYR:CD2	2.96	0.43
1:C:228:MET:CG	1:C:232:PHE:CZ	3.02	0.43
1:C:287:LYS:HD3	1:C:310:ASP:OD2	2.17	0.43
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.18	0.43
1:A:171:ILE:HG12	1:A:176:LEU:HD23	2.00	0.43
1:A:312:PRO:O	1:A:314:LYS:N	2.52	0.43
1:B:275:LEU:C	1:B:275:LEU:CD2	2.92	0.43
1:D:67:ARG:HH11	1:D:67:ARG:HG3	1.84	0.43
1:A:354:LEU:HD21	1:A:379:ASN:HB3	2.00	0.43
1:A:387:ARG:O	1:A:390:ARG:N	2.52	0.43
1:A:412:LEU:O	1:A:413:GLU:C	2.62	0.43
1:B:276:THR:O	1:B:277:ILE:C	2.60	0.43
1:B:354:LEU:HD11	1:B:381:VAL:HG12	2.01	0.43
1:C:197:PHE:O	1:C:201:ILE:HG12	2.17	0.43
1:D:112:LEU:CB	1:D:192:MET:HE1	2.41	0.43
1:D:282:ILE:HG23	1:D:352:TYR:HB2	2.01	0.43
1:D:316:ARG:NH1	1:D:316:ARG:CG	2.80	0.43
1:A:187:ASP:HA	1:A:217:ILE:HB	2.00	0.43
1:C:116:ARG:CG	1:C:141:ILE:HG21	2.49	0.43
1:D:264:LYS:HB3	1:D:352:TYR:CE1	2.54	0.43
1:D:360:LEU:HD12	1:D:361:TYR:N	2.32	0.43
1:A:187:ASP:O	1:A:188:GLU:C	2.62	0.42
1:A:339:ARG:HG3	1:A:339:ARG:HH11	1.83	0.42
1:B:362:ILE:C	1:B:364:ARG:H	2.26	0.42
1:B:385:ASP:O	1:B:387:ARG:N	2.52	0.42
1:C:145:ASN:OD1	1:C:148:GLU:HB3	2.18	0.42
1:B:233:MET:HG2	1:B:236:PRO:HB3	2.01	0.42
1:C:362:ILE:C	1:C:364:ARG:N	2.76	0.42
1:D:290:VAL:O	1:D:291:ASP:C	2.61	0.42
1:D:315:GLU:O	1:D:316:ARG:C	2.62	0.42
1:D:390:ARG:O	1:D:394:GLN:HG2	2.19	0.42
1:B:265:PHE:O	1:B:266:ASP:C	2.61	0.42
1:C:48:ASP:OD1	1:C:48:ASP:N	2.52	0.42
1:C:51:ARG:HD3	1:C:132:TYR:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLY:C	1:C:89:THR:H	2.26	0.42
1:C:101:ASP:H	1:C:108:GLN:HE22	1.67	0.42
1:C:290:VAL:O	1:C:291:ASP:C	2.61	0.42
1:D:120:VAL:O	1:D:123:GLN:HB3	2.20	0.42
1:A:387:ARG:C	1:A:389:LEU:N	2.76	0.42
1:B:320:MET:C	1:B:322:GLU:N	2.77	0.42
1:C:187:ASP:HA	1:C:217:ILE:HB	2.00	0.42
1:C:297:MET:O	1:C:302:PHE:HB2	2.19	0.42
1:D:111:ILE:C	1:D:112:LEU:HD23	2.45	0.42
1:D:272:TYR:CE2	1:D:302:PHE:CD1	3.07	0.42
1:D:336:VAL:O	1:D:337:TRP:CG	2.72	0.42
1:D:362:ILE:HG23	1:D:363:HIS:N	2.34	0.42
1:B:43:MET:CE	1:B:66:GLN:HG3	2.48	0.42
1:B:88:LYS:HD2	1:B:88:LYS:HA	1.92	0.42
1:B:246:LEU:HB3	1:B:362:ILE:HD11	1.99	0.42
1:C:361:TYR:O	1:C:365:ILE:HG12	2.20	0.42
1:D:116:ARG:CG	1:D:141:ILE:HG21	2.49	0.42
1:D:254:PHE:HA	1:D:401:ASP:O	2.19	0.42
1:D:319:ILE:O	1:D:320:MET:C	2.63	0.42
1:A:396:TYR:O	1:A:397:SER:C	2.62	0.42
1:B:281:VAL:HG22	1:B:331:LEU:HD23	2.01	0.42
1:B:335:ASP:OD1	1:B:363:HIS:CE1	2.73	0.42
1:C:269:CYS:O	1:C:272:TYR:N	2.46	0.42
1:D:120:VAL:O	1:D:121:GLN:C	2.62	0.42
1:D:191:GLU:O	1:D:192:MET:C	2.63	0.42
1:D:360:LEU:HA	1:D:363:HIS:HB3	2.00	0.42
1:D:402:GLU:O	1:D:404:PRO:HD3	2.20	0.42
1:A:118:LEU:O	1:A:122:ILE:HG13	2.19	0.42
1:A:360:LEU:HA	1:A:363:HIS:CB	2.49	0.42
1:A:360:LEU:CA	1:A:363:HIS:HB3	2.50	0.42
1:B:191:GLU:O	1:B:192:MET:C	2.63	0.42
1:B:269:CYS:O	1:B:270:ASP:C	2.62	0.42
1:C:233:MET:HG2	1:C:236:PRO:HB3	2.01	0.42
1:C:274:THR:CA	1:C:277:ILE:HG13	2.48	0.42
1:D:171:ILE:CG1	1:D:176:LEU:HD23	2.49	0.42
1:D:275:LEU:C	1:D:275:LEU:CD2	2.92	0.42
1:D:334:THR:OG1	1:D:336:VAL:CG1	2.61	0.42
1:A:154:ASP:C	1:A:156:GLY:N	2.73	0.42
1:A:171:ILE:CD1	1:A:204:VAL:HG13	2.50	0.42
1:B:395:TYR:C	1:B:397:SER:H	2.28	0.42
1:C:359:GLU:HA	1:C:359:GLU:OE1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:VAL:O	1:D:337:TRP:CD2	2.73	0.42
1:D:407:VAL:C	1:D:409:ASP:H	2.28	0.42
1:A:285:ASN:OD1	1:A:353:ASP:HB3	2.20	0.42
1:B:69:ILE:O	1:B:70:LYS:C	2.61	0.42
1:B:171:ILE:HG12	1:B:176:LEU:HD23	2.02	0.42
1:B:265:PHE:CE1	1:B:269:CYS:SG	3.13	0.42
1:B:272:TYR:O	1:B:273:ASP:C	2.63	0.42
1:C:106:GLU:O	1:C:108:GLN:HG3	2.20	0.42
1:A:51:ARG:HD3	1:A:132:TYR:CD2	2.54	0.42
1:A:403:MET:HA	1:A:404:PRO:HD3	1.79	0.42
1:B:171:ILE:CD1	1:B:204:VAL:HG13	2.50	0.42
1:B:246:LEU:CD1	1:B:341:LEU:HG	2.50	0.42
1:C:410:LEU:O	1:C:410:LEU:HD23	2.20	0.42
1:D:335:ASP:OD2	1:D:364:ARG:HD3	2.20	0.42
1:A:172:ARG:C	1:A:174:ARG:H	2.27	0.41
1:A:226:LEU:HA	1:A:229:THR:OG1	2.20	0.41
1:C:69:ILE:O	1:C:70:LYS:C	2.62	0.41
1:C:116:ARG:O	1:C:117:GLU:C	2.63	0.41
1:C:136:GLN:O	1:C:158:HIS:HB2	2.20	0.41
1:C:216:LEU:C	1:C:216:LEU:CD2	2.92	0.41
1:C:226:LEU:HA	1:C:229:THR:OG1	2.20	0.41
1:D:233:MET:HG2	1:D:236:PRO:HB3	2.01	0.41
1:A:312:PRO:C	1:A:314:LYS:N	2.78	0.41
1:B:67:ARG:O	1:B:68:ALA:C	2.63	0.41
1:B:255:PHE:CD2	1:B:400:ILE:HG22	2.53	0.41
1:B:309:GLY:C	1:B:311:MET:N	2.77	0.41
1:D:40:PHE:CZ	1:D:58:PHE:CD2	3.08	0.41
1:D:404:PRO:C	1:D:406:ASN:H	2.28	0.41
1:A:111:ILE:C	1:A:112:LEU:HD23	2.45	0.41
1:A:274:THR:O	1:A:274:THR:CG2	2.67	0.41
1:A:343:VAL:O	1:A:344:PRO:C	2.62	0.41
1:B:272:TYR:CZ	1:B:302:PHE:HD1	2.38	0.41
1:B:274:THR:HA	1:B:277:ILE:HG13	2.03	0.41
1:A:265:PHE:O	1:A:266:ASP:C	2.62	0.41
1:A:319:ILE:O	1:A:322:GLU:HB2	2.21	0.41
1:B:282:ILE:HG12	1:B:350:ILE:HB	2.02	0.41
1:B:360:LEU:HD12	1:B:360:LEU:O	2.19	0.41
1:C:171:ILE:CD1	1:C:204:VAL:HG13	2.49	0.41
1:C:252:LYS:HB2	1:C:376:VAL:HG22	2.02	0.41
1:C:253:GLN:HE22	1:C:398:THR:HG21	1.85	0.41
1:C:345:GLN:O	1:C:345:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PHE:CZ	1:D:58:PHE:HD2	2.39	0.41
1:A:88:LYS:HD2	1:A:88:LYS:HA	1.92	0.41
1:A:265:PHE:CE1	1:A:269:CYS:SG	3.13	0.41
1:B:210:PRO:O	1:B:211:ALA:CB	2.64	0.41
1:B:343:VAL:HG23	1:B:343:VAL:O	2.20	0.41
1:D:139:ALA:HA	1:D:161:ALA:O	2.20	0.41
1:D:187:ASP:HA	1:D:217:ILE:HB	2.03	0.41
1:D:265:PHE:CE1	1:D:269:CYS:SG	3.13	0.41
1:B:155:TYR:O	1:B:155:TYR:CD1	2.74	0.41
1:C:265:PHE:CE1	1:C:269:CYS:SG	3.13	0.41
1:D:226:LEU:HA	1:D:229:THR:OG1	2.20	0.41
1:D:279:GLN:HB3	1:D:323:PHE:CZ	2.55	0.41
1:D:305:SER:O	1:D:331:LEU:HD12	2.21	0.41
1:A:87:GLY:C	1:A:89:THR:H	2.29	0.41
1:B:406:ASN:C	1:B:408:ALA:N	2.78	0.41
1:C:62:SER:HB3	1:C:65:GLN:CD	2.45	0.41
1:D:275:LEU:HD21	1:D:330:VAL:HG23	1.99	0.41
1:D:386:ILE:HD12	1:D:386:ILE:HA	1.88	0.41
1:A:130:GLY:O	1:A:131:ASP:C	2.62	0.41
1:C:341:LEU:HD12	1:C:341:LEU:N	2.29	0.41
1:D:390:ARG:HD2	1:D:390:ARG:HA	1.79	0.41
1:A:191:GLU:O	1:A:192:MET:C	2.63	0.41
1:A:281:VAL:HG23	1:A:346:VAL:HG11	2.02	0.41
1:B:79:ILE:HD13	1:B:229:THR:HG21	2.02	0.41
1:B:87:GLY:C	1:B:89:THR:N	2.79	0.41
1:B:226:LEU:HA	1:B:229:THR:OG1	2.20	0.41
1:B:320:MET:HA	1:B:320:MET:CE	2.39	0.41
1:C:164:PRO:HB2	1:C:197:PHE:CD2	2.53	0.41
1:C:367:ARG:HH12	1:C:369:GLY:HA2	1.85	0.41
1:D:40:PHE:CE2	1:D:58:PHE:HD2	2.38	0.41
1:D:40:PHE:HZ	1:D:58:PHE:CE2	2.38	0.41
1:D:90:ALA:O	1:D:91:THR:C	2.64	0.41
1:D:337:TRP:CG	1:D:342:ASP:O	2.74	0.41
1:A:74:LYS:HD2	1:A:317:GLU:OE2	2.21	0.41
1:A:367:ARG:CZ	1:A:369:GLY:HA2	2.51	0.41
1:B:64:ILE:CG1	1:B:65:GLN:N	2.84	0.41
1:C:203:ASP:O	1:C:206:ARG:HB3	2.20	0.41
1:C:203:ASP:HA	1:C:206:ARG:HB2	2.01	0.41
1:D:362:ILE:HB	1:D:396:TYR:CZ	2.55	0.41
1:A:362:ILE:HB	1:A:396:TYR:CZ	2.56	0.40
1:B:141:ILE:HD11	1:B:163:THR:OG1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ILE:HD12	1:C:64:ILE:C	2.46	0.40
1:C:87:GLY:C	1:C:89:THR:N	2.77	0.40
1:C:406:ASN:C	1:C:408:ALA:H	2.27	0.40
1:D:344:PRO:O	1:D:345:GLN:C	2.63	0.40
1:A:136:GLN:O	1:A:158:HIS:HB2	2.21	0.40
1:A:381:VAL:HG11	1:A:389:LEU:HD13	2.02	0.40
1:B:313:GLN:HA	1:B:316:ARG:HG3	2.02	0.40
1:C:116:ARG:HG3	1:C:116:ARG:NH1	2.34	0.40
1:C:187:ASP:O	1:C:188:GLU:C	2.63	0.40
1:D:362:ILE:HD13	1:D:362:ILE:C	2.46	0.40
1:A:174:ARG:HG2	1:A:174:ARG:NH1	2.35	0.40
1:B:319:ILE:O	1:B:320:MET:C	2.65	0.40
1:C:360:LEU:C	1:C:362:ILE:N	2.79	0.40
1:D:289:LYS:HD3	1:D:353:ASP:OD1	2.22	0.40
1:D:385:ASP:C	1:D:387:ARG:N	2.78	0.40
1:A:143:GLY:C	1:A:145:ASN:N	2.79	0.40
1:A:232:PHE:CD2	1:A:232:PHE:N	2.89	0.40
1:B:320:MET:O	1:B:322:GLU:N	2.54	0.40
1:C:335:ASP:OD1	1:C:363:HIS:CE1	2.74	0.40
1:C:344:PRO:O	1:C:345:GLN:C	2.63	0.40
1:D:312:PRO:HG2	1:D:315:GLU:HB3	2.02	0.40
1:A:105:ARG:NH1	1:A:155:TYR:CE1	2.90	0.40
1:A:314:LYS:O	1:A:318:SER:HB2	2.22	0.40
1:C:269:CYS:O	1:C:270:ASP:C	2.65	0.40
1:C:410:LEU:C	1:C:412:LEU:N	2.80	0.40
1:D:216:LEU:C	1:D:216:LEU:CD2	2.92	0.40
1:D:272:TYR:CD2	1:D:302:PHE:HE1	2.40	0.40
1:D:272:TYR:CE1	1:D:275:LEU:HD22	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ARG:NH2	1:B:326:GLY:O[2_555]	2.10	0.10

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	374/391 (96%)	309 (83%)	55 (15%)	10 (3%)	4	22
1	B	374/391 (96%)	297 (79%)	68 (18%)	9 (2%)	4	24
1	C	374/391 (96%)	303 (81%)	62 (17%)	9 (2%)	4	24
1	D	374/391 (96%)	300 (80%)	64 (17%)	10 (3%)	4	22
All	All	1496/1564 (96%)	1209 (81%)	249 (17%)	38 (2%)	4	23

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ILE
1	A	406	ASN
1	B	141	ILE
1	B	310	ASP
1	C	141	ILE
1	D	141	ILE
1	A	179	ARG
1	A	313	GLN
1	A	342	ASP
1	A	357	ASN
1	A	358	ARG
1	B	179	ARG
1	B	335	ASP
1	B	406	ASN
1	C	179	ARG
1	C	316	ARG
1	D	179	ARG
1	D	211	ALA
1	D	345	GLN
1	D	405	MET
1	C	358	ARG
1	C	411	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	103	GLN
1	D	342	ASP
1	A	103	GLN
1	A	210	PRO
1	B	103	GLN
1	B	369	GLY
1	B	384	ASP
1	C	103	GLN
1	B	344	PRO
1	C	322	GLU
1	D	383	ASN
1	C	301	ASN
1	D	369	GLY
1	C	326	GLY
1	A	146	VAL
1	D	146	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	331/346 (96%)	298 (90%)	33 (10%)	7	27
1	B	331/346 (96%)	299 (90%)	32 (10%)	8	28
1	C	331/346 (96%)	295 (89%)	36 (11%)	6	23
1	D	331/346 (96%)	297 (90%)	34 (10%)	7	25
All	All	1324/1384 (96%)	1189 (90%)	135 (10%)	7	26

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	82	SER
1	A	84	SER
1	A	141	ILE
1	A	166	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	ARG
1	A	191	GLU
1	A	192	MET
1	A	200	GLN
1	A	210	PRO
1	A	223	HIS
1	A	224	GLU
1	A	227	GLU
1	A	232	PHE
1	A	240	LEU
1	A	246	LEU
1	A	248	LEU
1	A	249	GLU
1	A	260	ARG
1	A	275	LEU
1	A	276	THR
1	A	277	ILE
1	A	278	THR
1	A	324	ARG
1	A	341	LEU
1	A	345	GLN
1	A	354	LEU
1	A	360	LEU
1	A	362	ILE
1	A	364	ARG
1	A	378	ILE
1	A	386	ILE
1	A	403	MET
1	B	64	ILE
1	B	82	SER
1	B	84	SER
1	B	141	ILE
1	B	166	ARG
1	B	172	ARG
1	B	191	GLU
1	B	192	MET
1	B	200	GLN
1	B	223	HIS
1	B	224	GLU
1	B	227	GLU
1	B	232	PHE
1	B	240	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	246	LEU
1	B	248	LEU
1	B	249	GLU
1	B	260	ARG
1	B	275	LEU
1	B	276	THR
1	B	278	THR
1	B	303	THR
1	B	307	MET
1	B	324	ARG
1	B	325	SER
1	B	329	ARG
1	B	347	SER
1	B	354	LEU
1	B	360	LEU
1	B	362	ILE
1	B	386	ILE
1	B	398	THR
1	C	64	ILE
1	C	82	SER
1	C	84	SER
1	C	141	ILE
1	C	166	ARG
1	C	172	ARG
1	C	191	GLU
1	C	192	MET
1	C	200	GLN
1	C	206	ARG
1	C	223	HIS
1	C	224	GLU
1	C	227	GLU
1	C	232	PHE
1	C	240	LEU
1	C	246	LEU
1	C	248	LEU
1	C	249	GLU
1	C	260	ARG
1	C	271	LEU
1	C	273	ASP
1	C	275	LEU
1	C	276	THR
1	C	278	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	303	THR
1	C	305	SER
1	C	343	VAL
1	C	358	ARG
1	C	359	GLU
1	C	360	LEU
1	C	362	ILE
1	C	363	HIS
1	C	364	ARG
1	C	397	SER
1	C	405	MET
1	C	413	GLU
1	D	64	ILE
1	D	82	SER
1	D	84	SER
1	D	141	ILE
1	D	166	ARG
1	D	172	ARG
1	D	191	GLU
1	D	192	MET
1	D	200	GLN
1	D	223	HIS
1	D	224	GLU
1	D	227	GLU
1	D	232	PHE
1	D	240	LEU
1	D	246	LEU
1	D	248	LEU
1	D	249	GLU
1	D	260	ARG
1	D	275	LEU
1	D	276	THR
1	D	278	THR
1	D	301	ASN
1	D	303	THR
1	D	307	MET
1	D	325	SER
1	D	330	VAL
1	D	343	VAL
1	D	358	ARG
1	D	360	LEU
1	D	362	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	364	ARG
1	D	381	VAL
1	D	398	THR
1	D	403	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	123	GLN
1	A	200	GLN
1	A	213	GLN
1	A	253	GLN
1	A	301	ASN
1	A	345	GLN
1	A	394	GLN
1	B	103	GLN
1	B	108	GLN
1	B	123	GLN
1	B	200	GLN
1	B	213	GLN
1	B	301	ASN
1	B	308	HIS
1	B	313	GLN
1	B	345	GLN
1	B	356	ASN
1	C	103	GLN
1	C	108	GLN
1	C	123	GLN
1	C	200	GLN
1	C	213	GLN
1	C	253	GLN
1	C	285	ASN
1	C	301	ASN
1	C	345	GLN
1	C	363	HIS
1	C	394	GLN
1	D	103	GLN
1	D	108	GLN
1	D	123	GLN
1	D	200	GLN
1	D	213	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	285	ASN
1	D	301	ASN
1	D	308	HIS
1	D	394	GLN

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	376/391 (96%)	0.51	38 (10%)	12 10	4, 45, 113, 151	0
1	B	376/391 (96%)	0.67	50 (13%)	7 6	6, 52, 129, 173	0
1	C	376/391 (96%)	0.52	34 (9%)	15 11	3, 49, 126, 165	0
1	D	376/391 (96%)	0.83	61 (16%)	4 4	9, 62, 135, 156	0
All	All	1504/1564 (96%)	0.63	183 (12%)	8 7	3, 51, 127, 173	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	ILE	6.7
1	D	56	TYR	6.0
1	B	277	ILE	5.6
1	D	299	GLU	5.5
1	D	274	THR	5.5
1	A	273	ASP	5.3
1	D	272	TYR	5.2
1	D	59	GLU	5.0
1	B	272	TYR	5.0
1	A	412	LEU	4.8
1	C	407	VAL	4.7
1	C	59	GLU	4.6
1	D	302	PHE	4.6
1	D	58	PHE	4.5
1	A	297	MET	4.4
1	B	274	THR	4.4
1	D	262	GLU	4.3
1	C	303	THR	4.2
1	A	274	THR	4.2
1	D	250	GLY	4.2
1	B	105	ARG	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	87	GLY	4.1
1	B	410	LEU	4.1
1	A	411	ILE	4.1
1	D	257	ALA	4.0
1	C	357	ASN	4.0
1	B	412	LEU	4.0
1	B	250	GLY	4.0
1	D	407	VAL	3.9
1	C	412	LEU	3.9
1	D	340	GLY	3.9
1	D	210	PRO	3.9
1	A	88	LYS	3.8
1	C	277	ILE	3.8
1	B	88	LYS	3.7
1	D	411	ILE	3.7
1	C	411	ILE	3.7
1	C	154	ASP	3.7
1	C	56	TYR	3.6
1	C	141	ILE	3.6
1	A	410	LEU	3.6
1	D	412	LEU	3.5
1	D	300	ALA	3.4
1	A	59	GLU	3.4
1	C	274	THR	3.4
1	B	210	PRO	3.4
1	D	38	PRO	3.4
1	B	302	PHE	3.4
1	D	410	LEU	3.3
1	C	105	ARG	3.3
1	B	335	ASP	3.3
1	D	356	ASN	3.3
1	B	407	VAL	3.3
1	C	88	LYS	3.3
1	B	373	ARG	3.3
1	C	373	ARG	3.3
1	D	273	ASP	3.3
1	A	408	ALA	3.2
1	D	140	CYS	3.2
1	B	276	THR	3.2
1	D	60	LYS	3.1
1	B	211	ALA	3.1
1	B	257	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	271	LEU	3.1
1	A	303	THR	3.1
1	C	250	GLY	3.0
1	D	298	ARG	3.0
1	D	329	ARG	3.0
1	D	341	LEU	3.0
1	B	177	ARG	3.0
1	C	410	LEU	3.0
1	C	316	ARG	3.0
1	B	275	LEU	2.9
1	D	338	ALA	2.9
1	A	409	ASP	2.9
1	D	337	TRP	2.9
1	B	141	ILE	2.9
1	B	357	ASN	2.8
1	C	143	GLY	2.8
1	D	408	ALA	2.8
1	B	278	THR	2.8
1	A	292	TRP	2.8
1	D	357	ASN	2.8
1	A	272	TYR	2.8
1	B	154	ASP	2.8
1	D	154	ASP	2.7
1	B	298	ARG	2.7
1	C	152	LYS	2.7
1	B	256	VAL	2.7
1	B	315	GLU	2.7
1	C	272	TYR	2.7
1	D	344	PRO	2.7
1	C	174	ARG	2.7
1	D	88	LYS	2.7
1	D	335	ASP	2.7
1	A	358	ARG	2.7
1	A	141	ILE	2.6
1	B	142	GLY	2.6
1	B	284	CYS	2.6
1	C	223	HIS	2.6
1	B	408	ALA	2.6
1	C	38	PRO	2.6
1	B	273	ASP	2.5
1	C	370	ARG	2.5
1	B	338	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	150	ILE	2.5
1	B	403	MET	2.5
1	A	138	HIS	2.5
1	A	207	TYR	2.5
1	D	176	LEU	2.5
1	B	271	LEU	2.5
1	B	143	GLY	2.5
1	A	224	GLU	2.5
1	A	308	HIS	2.5
1	B	59	GLU	2.4
1	A	296	LYS	2.4
1	B	292	TRP	2.4
1	D	168	PHE	2.4
1	A	58	PHE	2.4
1	B	223	HIS	2.4
1	B	345	GLN	2.4
1	B	413	GLU	2.4
1	B	260	ARG	2.4
1	A	317	GLU	2.4
1	B	300	ALA	2.3
1	D	301	ASN	2.3
1	A	283	PHE	2.3
1	A	373	ARG	2.3
1	C	142	GLY	2.3
1	C	271	LEU	2.3
1	A	84	SER	2.3
1	D	275	LEU	2.3
1	D	169	ASP	2.3
1	B	60	LYS	2.3
1	D	51	ARG	2.3
1	D	278	THR	2.3
1	B	384	ASP	2.3
1	B	117	GLU	2.3
1	D	386	ILE	2.3
1	D	207	TYR	2.3
1	A	370	ARG	2.3
1	A	262	GLU	2.2
1	A	250	GLY	2.2
1	C	85	GLY	2.2
1	A	146	VAL	2.2
1	A	136	GLN	2.2
1	B	227	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	141	ILE	2.2
1	C	58	PHE	2.2
1	D	370	ARG	2.2
1	A	83	GLN	2.2
1	C	299	GLU	2.2
1	D	227	GLU	2.2
1	C	140	CYS	2.2
1	D	166	ARG	2.1
1	B	140	CYS	2.1
1	D	345	GLN	2.1
1	A	309	GLY	2.1
1	D	145	ASN	2.1
1	A	223	HIS	2.1
1	B	61	PRO	2.1
1	B	301	ASN	2.1
1	D	256	VAL	2.1
1	A	177	ARG	2.1
1	D	174	ARG	2.1
1	D	170	MET	2.1
1	D	361	TYR	2.1
1	A	38	PRO	2.1
1	D	224	GLU	2.1
1	C	266	ASP	2.1
1	C	345	GLN	2.1
1	D	175	SER	2.0
1	A	263	TRP	2.0
1	A	86	THR	2.0
1	D	139	ALA	2.0
1	B	326	GLY	2.0
1	B	224	GLU	2.0
1	C	60	LYS	2.0
1	B	205	TYR	2.0
1	A	227	GLU	2.0
1	D	413	GLU	2.0
1	D	316	ARG	2.0
1	C	354	LEU	2.0

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

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.