



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:16 AM UTC

PDB ID : 3HVT / pdb_00003hvt
Title : STRUCTURAL BASIS OF ASYMMETRY IN THE HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE HETEROODIMER
Authors : Steitz, T.A.; Smerdon, S.J.; Jaeger, J.; Wang, J.; Kohlstaedt, L.A.; Chirino, A.J.; Friedman, J.M.; Rice, P.A.
Deposited on : 1994-07-25
Resolution : 2.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

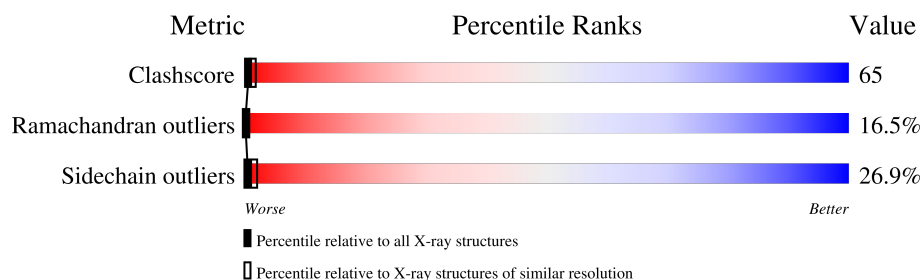
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

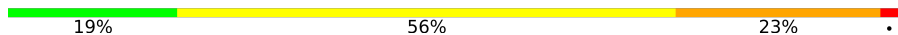
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	 19% 56% 23% •
2	B	428	 20% 37% 25% 11% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7426 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.

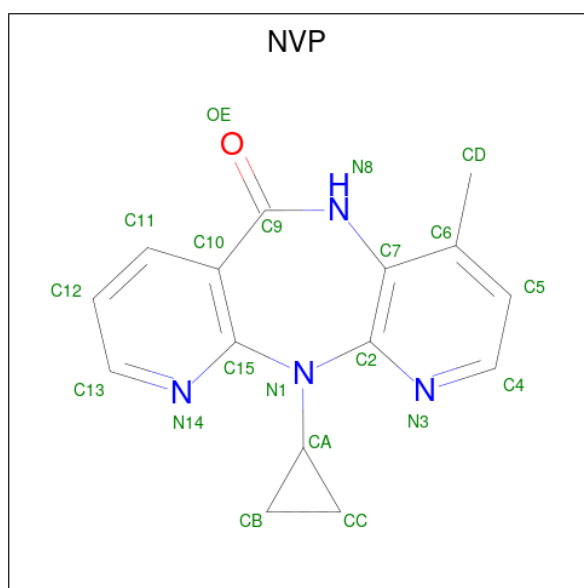
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4248	2744	709	787	8			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	398	Total	C	N	O	S	0	0	0
			3158	2050	523	579	6			

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (CCD ID: NVP) (formula: C₁₅H₁₄N₄O).



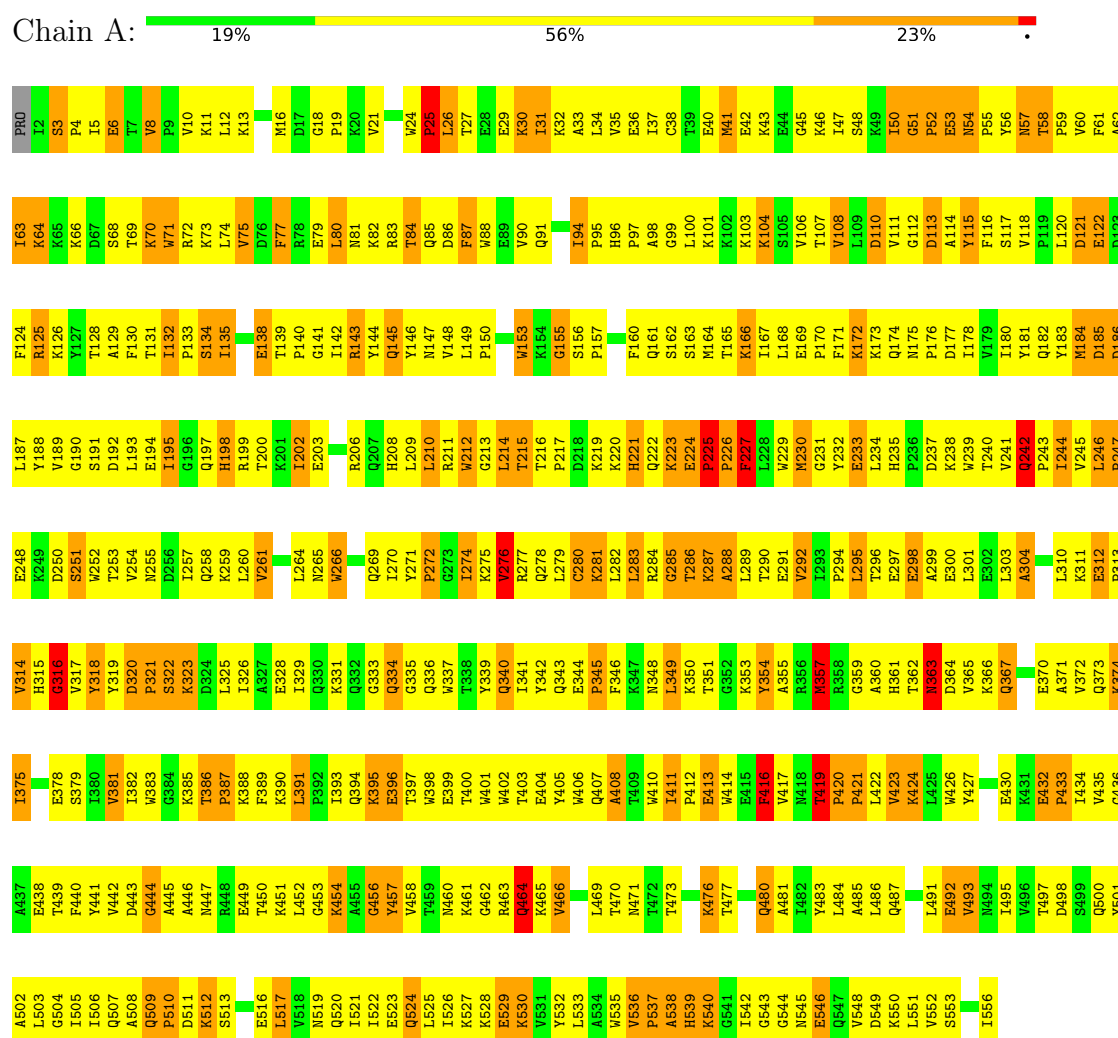
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

3 Residue-property plots

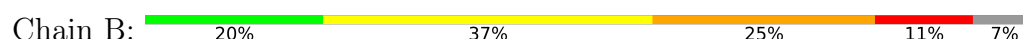
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)



L391	H315	V254	E194	T131	I63	PRO
P392	G316	N255	I195	I132	K64	I2
I393	V317	D256	G196	P133	K65	S3
Q394	P321	I257	Q197	S134	K66	P4
K395	S322	Q258	H198	T135	D67	I5
E396	K323	K259	R199	N136	S68	E6
T397	Q332	L260	T200		T69	V7
W398	Q333	V261	K201	P140	K70	T8
W401	G334	G262	L202	G141	W71	P9
W402	Q334	K263	E203	I142	R72	V10
T403	G335	N265	E204	R143	K73	K11
E404	W336	W266	L205	Y144	L74	L12
Y405	W337	A267	R206	Q145	V75	K13
W406	Q340	S268	Q207	Y146	D76	P14
Q407		Q269	H208	M147	F77	G15
A408	Q340	I270	L209	V148	R78	M16
T409	E344	I271	L210	L149	E79	D17
W410	P345	Y271	R211	P150	L80	
I411	F346	G272	W212	Q151	N81	V21
P412	K347	T273	G213	G152	K82	K22
E413		I274	L214	W153	R83	Q23
W414	K350	K275	T215	K154	T84	W24
E415		V276	T216	G155	Q85	P25
F416	K353	R277	P217	S156	D86	L26
W417	Y354	Q278	D218	P157	F87	T27
N418	A355	L279	K219	A158	W88	E28
T419		C280	K220	I159	E89	E29
P420	K358	K281	H221	F160	V90	K30
P421	GLY	L282	Q222	Q161	Q91	I31
L422	ALA	L283	K223	S162	L92	K32
V423	HIS	G284	E224	S163	G93	A33
K424	THR	R285	P225	M164	I94	L34
L425	ASN	T286	PRO	T165	P95	V35
W426	D364	K287	PHE	K166		E36
Y427	V365	A288	LEU	I167	G99	T37
Q428	K366	L289	TRP	L168	L100	C38
	Q367	T290	MET	E169	T39	
	L368	E291	GLY	P170	K102	E40
	T369	V292	TYR	F171	K103	N41
	E370	L293	GLU	K172	K104	E42
	A371	P294	LEU	K173	S105	K43
	V372	L295	HIS	Q174	V106	E44
	Q373	T296	PRO	N175	T107	G45
	K374	E297	ASP	P176	V108	K46
	I375	E298	LYS	D177	K46	I47
	T376	A299	TRP	I178	Y115	S48
	T377	E300	THR	V179	F116	K49
	E378	L301	VAL	I180	S117	T50
	S379	E302	GLN		V118	G51
	I380	L303	PRO	Y183	P119	P52
	V381	A304	ILE	M184	L120	E53
	I382	N306	VAL	D185	D121	N54
	W383	R307	LEU	D186	E122	P55
		E308	PRO	L187	D123	Y56
		I309	GLU	Y188	F124	N57
			LYS	V189	R125	T58
			D250	G190		P59
			S251	S191	T128	V60
			W252	D192	A129	F61
			P313	T244	F142	A62

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.60 Å 69.90 Å 105.50 Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.266 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7426	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NVP

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	0.98	9/4358 (0.2%)	1.60	103/5951 (1.7%)
2	B	1.05	5/3242 (0.2%)	1.62	100/4411 (2.3%)
All	All	1.01	14/7600 (0.2%)	1.61	203/10362 (2.0%)

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
2	B	0	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	419	THR	CA-CB	11.80	1.60	1.52
2	B	142	ILE	CA-CB	8.52	1.62	1.54
1	A	357	MET	SD-CE	7.90	1.99	1.79
2	B	277	ARG	C-O	6.76	1.31	1.24
1	A	94	ILE	CA-CB	6.33	1.62	1.54
1	A	420	PRO	CA-C	6.04	1.57	1.52
2	B	150	PRO	CA-C	-5.75	1.47	1.52
1	A	108	VAL	CA-CB	5.62	1.62	1.54
1	A	41	MET	SD-CE	5.46	1.93	1.79
1	A	90	VAL	CA-CB	5.36	1.60	1.54
1	A	381	VAL	CA-CB	-5.31	1.48	1.54
2	B	296	THR	CA-CB	5.27	1.62	1.53
1	A	276	VAL	CA-C	5.27	1.59	1.52
1	A	8	VAL	CA-C	5.21	1.57	1.53

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	288	ALA	N-CA-C	17.82	133.10	110.65
2	B	178	ILE	N-CA-C	-14.56	87.15	108.12
1	A	24	TRP	CA-C-N	14.07	137.43	119.84
1	A	24	TRP	C-N-CA	14.07	137.43	119.84
1	A	51	GLY	CA-C-N	12.67	132.62	119.19
1	A	51	GLY	C-N-CA	12.67	132.62	119.19
1	A	420	PRO	CA-C-N	12.36	135.29	119.84
1	A	420	PRO	C-N-CA	12.36	135.29	119.84
1	A	202	ILE	N-CA-C	-12.05	101.44	111.81
1	A	274	ILE	N-CA-C	-11.82	96.85	110.21
2	B	303	LEU	N-CA-C	-11.60	98.62	111.14
2	B	402	TRP	N-CA-C	-11.41	98.84	111.28
1	A	374	LYS	N-CA-C	-10.83	99.78	113.43
2	B	279	LEU	N-CA-C	-10.46	97.91	112.45
1	A	225	PRO	N-CA-C	10.23	123.18	110.70
2	B	258	GLN	N-CA-C	-10.14	100.23	111.28
2	B	222	GLN	N-CA-C	9.99	125.28	109.39
1	A	58	THR	CA-C-N	9.93	132.26	119.84
1	A	58	THR	C-N-CA	9.93	132.26	119.84
2	B	104	LYS	N-CA-C	9.84	131.76	110.80
1	A	388	LYS	N-CA-C	-9.63	96.22	110.48
1	A	335	GLY	N-CA-C	-9.52	102.06	115.30
1	A	85	GLN	N-CA-C	9.51	131.05	110.80
2	B	54	ASN	CA-C-N	9.42	131.61	119.84
2	B	54	ASN	C-N-CA	9.42	131.61	119.84
1	A	480	GLN	N-CA-C	-9.26	101.06	111.71
1	A	517	LEU	N-CA-C	-9.22	100.79	111.03
1	A	375	ILE	N-CA-C	-9.21	101.77	110.42
1	A	224	GLU	CA-C-N	9.18	129.84	120.38
1	A	224	GLU	C-N-CA	9.18	129.84	120.38
2	B	365	VAL	N-CA-C	-9.13	101.50	110.72
2	B	419	THR	C-N-CD	-8.95	100.92	120.60
1	A	166	LYS	N-CA-C	-8.93	97.89	111.56
2	B	276	VAL	CA-C-N	8.87	133.12	120.79
2	B	276	VAL	C-N-CA	8.87	133.12	120.79
2	B	198	HIS	N-CA-C	-8.75	92.16	110.80
1	A	280	CYS	N-CA-C	-8.64	102.11	114.12
1	A	52	PRO	N-CA-C	8.63	124.87	113.57
1	A	90	VAL	N-CA-C	8.52	120.57	109.58
1	A	132	ILE	N-CA-C	-8.52	98.02	107.73
2	B	267	ALA	N-CA-C	-8.48	101.61	111.03
2	B	389	PHE	N-CA-C	8.45	122.79	110.28
2	B	345	PRO	N-CA-CB	8.30	111.97	103.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	GLU	N-CA-C	-8.30	97.59	109.96
2	B	354	TYR	N-CA-C	-8.28	99.86	110.53
1	A	303	LEU	N-CA-C	-8.23	101.00	112.45
1	A	313	PRO	N-CA-CB	8.23	111.89	103.25
2	B	120	LEU	N-CA-C	8.23	120.65	108.14
1	A	155	GLY	N-CA-C	-8.22	102.87	112.73
2	B	397	THR	N-CA-C	-8.19	103.30	113.20
1	A	219	LYS	N-CA-C	-8.16	100.64	110.44
2	B	74	LEU	N-CA-C	-8.10	93.60	108.02
1	A	135	ILE	N-CA-C	8.02	119.46	107.51
1	A	334	GLN	N-CA-C	-7.99	104.50	112.97
1	A	231	GLY	N-CA-C	-7.92	96.29	111.02
1	A	230	MET	N-CA-C	-7.81	94.80	108.23
1	A	298	GLU	N-CA-C	7.77	120.65	111.71
2	B	313	PRO	N-CA-C	7.77	124.00	113.98
1	A	132	ILE	CA-C-N	-7.65	111.88	119.76
1	A	132	ILE	C-N-CA	-7.65	111.88	119.76
2	B	177	ASP	N-CA-C	7.65	127.09	110.80
2	B	8	VAL	CA-C-N	7.63	129.38	119.84
2	B	8	VAL	C-N-CA	7.63	129.38	119.84
1	A	476	LYS	N-CA-C	-7.55	103.92	113.43
1	A	21	VAL	N-CA-C	7.55	119.50	107.73
2	B	215	THR	N-CA-C	-7.51	99.04	110.30
1	A	18	GLY	CA-C-N	7.51	129.22	119.84
1	A	18	GLY	C-N-CA	7.51	129.22	119.84
1	A	91	GLN	N-CA-C	-7.47	98.97	110.10
1	A	391	LEU	N-CA-C	7.45	120.42	109.62
1	A	276	VAL	N-CA-C	7.41	124.76	109.34
2	B	196	GLY	N-CA-C	-7.34	106.10	115.42
2	B	123	ASP	N-CA-CB	-7.29	105.85	114.17
2	B	94	ILE	CA-C-N	7.27	128.26	120.11
2	B	94	ILE	C-N-CA	7.27	128.26	120.11
1	A	508	ALA	N-CA-C	-7.25	104.31	113.01
1	A	251	SER	N-CA-C	-7.20	95.46	110.80
2	B	321	PRO	N-CA-CB	7.20	110.81	103.25
2	B	89	GLU	N-CA-C	-7.08	104.28	114.12
1	A	110	ASP	N-CA-C	-7.01	101.48	110.53
1	A	386	THR	CA-C-N	7.01	127.18	120.31
1	A	386	THR	C-N-CA	7.01	127.18	120.31
1	A	364	ASP	N-CA-C	-6.96	103.38	110.97
2	B	132	ILE	N-CA-C	-6.95	99.81	107.73
1	A	244	ILE	N-CA-C	6.85	119.75	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	ASN	CA-C-N	6.82	128.37	119.84
2	B	175	ASN	C-N-CA	6.82	128.37	119.84
2	B	315	HIS	N-CA-C	6.72	125.12	110.80
2	B	353	LYS	N-CA-C	6.72	119.36	108.41
1	A	80	LEU	N-CA-C	-6.68	103.09	111.11
2	B	426	TRP	N-CA-C	-6.67	96.59	110.80
1	A	320	ASP	N-CA-C	-6.64	99.74	109.50
2	B	275	LYS	N-CA-C	6.62	119.61	110.35
1	A	454	LYS	N-CA-C	6.59	119.20	107.80
2	B	321	PRO	N-CA-C	-6.56	98.95	112.47
1	A	198	HIS	N-CA-C	-6.54	104.24	111.82
2	B	379	SER	N-CA-C	-6.54	104.16	111.28
1	A	86	ASP	N-CA-C	-6.48	104.26	111.71
1	A	360	ALA	N-CA-C	-6.48	99.91	109.62
2	B	199	ARG	N-CA-C	-6.47	103.34	111.11
2	B	270	ILE	N-CA-C	-6.43	95.97	109.34
1	A	53	GLU	N-CA-C	6.42	118.90	107.80
1	A	432	GLU	CA-C-N	6.41	127.86	119.84
1	A	432	GLU	C-N-CA	6.41	127.86	119.84
2	B	22	LYS	N-CA-C	6.39	120.86	111.34
2	B	277	ARG	O-C-N	-6.34	115.30	122.08
2	B	391	LEU	N-CA-C	6.34	117.79	109.93
1	A	41	MET	N-CA-C	-6.33	105.54	113.20
1	A	153	TRP	N-CA-C	-6.33	97.33	110.80
2	B	398	TRP	N-CA-C	-6.30	104.54	112.93
1	A	26	LEU	N-CA-C	-6.30	102.11	111.81
1	A	500	GLN	N-CA-C	-6.28	103.72	112.45
2	B	299	ALA	N-CA-C	-6.28	98.51	108.30
2	B	83	ARG	N-CA-C	6.24	119.06	111.82
2	B	142	ILE	N-CA-C	6.23	119.62	109.78
2	B	368	LEU	N-CA-C	-6.23	103.64	111.11
1	A	45	GLY	N-CA-C	-6.21	98.46	113.18
2	B	177	ASP	CA-C-N	6.20	131.60	122.99
2	B	177	ASP	C-N-CA	6.20	131.60	122.99
1	A	138	GLU	N-CA-C	-6.17	102.10	110.68
2	B	11	LYS	N-CA-C	6.17	118.56	109.24
2	B	293	ILE	CA-C-N	6.15	141.75	127.00
2	B	293	ILE	C-N-CA	6.15	141.75	127.00
2	B	269	GLN	N-CA-C	-6.13	97.73	110.80
2	B	143	ARG	N-CA-C	6.11	119.78	109.76
1	A	400	THR	N-CA-C	6.07	117.90	111.28
2	B	51	GLY	C-N-CD	-6.05	100.21	125.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	TRP	N-CA-C	-6.01	103.90	111.11
1	A	316	GLY	N-CA-C	5.98	127.36	113.18
1	A	212	TRP	N-CA-C	-5.93	103.76	111.71
2	B	160	PHE	N-CA-C	5.92	120.02	113.21
2	B	88	TRP	CA-C-N	5.90	131.50	122.23
2	B	88	TRP	C-N-CA	5.90	131.50	122.23
2	B	344	GLU	CA-C-N	5.88	127.19	119.84
2	B	344	GLU	C-N-CA	5.88	127.19	119.84
1	A	25	PRO	N-CA-C	5.86	124.55	112.47
2	B	206	ARG	N-CA-C	-5.82	105.01	111.71
2	B	296	THR	N-CA-C	5.80	117.66	108.79
2	B	194	GLU	N-CA-C	-5.78	99.38	108.63
1	A	242	GLN	N-CA-C	5.75	122.51	109.81
2	B	293	ILE	C-N-CD	-5.73	108.00	120.60
1	A	387	PRO	N-CA-C	5.72	120.26	111.57
1	A	420	PRO	C-N-CD	-5.72	101.56	125.00
2	B	335	GLY	N-CA-C	-5.71	99.64	113.18
1	A	411	ILE	CA-C-N	5.71	126.51	120.11
1	A	411	ILE	C-N-CA	5.71	126.51	120.11
1	A	104	LYS	N-CA-C	-5.71	104.98	111.14
2	B	92	LEU	N-CA-C	-5.69	98.68	110.80
1	A	70	LYS	N-CA-C	5.69	118.72	108.48
1	A	68	SER	N-CA-C	5.67	115.01	108.49
1	A	355	ALA	N-CA-C	-5.66	100.46	109.96
2	B	382	ILE	N-CA-C	5.66	120.33	112.35
2	B	50	ILE	N-CA-C	5.64	117.75	109.63
2	B	216	THR	N-CA-C	5.63	120.90	108.73
2	B	62	ALA	N-CA-C	-5.59	100.58	109.59
2	B	44	GLU	N-CA-C	-5.58	105.67	113.37
1	A	359	GLY	N-CA-C	5.58	126.41	113.18
2	B	51	GLY	CA-C-N	5.50	126.72	119.84
2	B	51	GLY	C-N-CA	5.50	126.72	119.84
2	B	78	ARG	N-CA-C	5.46	117.93	111.33
2	B	40	GLU	N-CA-C	-5.44	105.35	111.28
1	A	84	THR	CB-CA-C	-5.44	99.60	110.42
1	A	367	GLN	N-CA-C	-5.42	105.40	112.23
1	A	50	ILE	N-CA-C	-5.41	102.60	109.58
2	B	94	ILE	N-CA-C	-5.41	102.19	107.55
1	A	61	PHE	N-CA-CB	-5.39	101.83	110.77
1	A	272	PRO	N-CA-C	5.33	119.23	111.03
2	B	80	LEU	N-CA-C	-5.33	105.64	111.82
2	B	367	GLN	N-CA-C	-5.33	105.59	112.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	PRO	N-CA-C	5.32	123.42	112.47
1	A	456	GLY	N-CA-C	5.31	125.77	113.18
2	B	340	GLN	N-CA-C	5.31	116.09	107.23
1	A	444	GLY	N-CA-C	-5.31	103.01	111.18
2	B	419	THR	CA-C-N	5.30	139.72	127.00
2	B	419	THR	C-N-CA	5.30	139.72	127.00
1	A	6	GLU	N-CA-C	5.30	117.60	107.75
2	B	277	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	318	TYR	N-CA-C	-5.29	106.86	113.15
2	B	195	ILE	N-CA-C	5.28	120.31	109.34
1	A	227	PHE	N-CA-C	5.27	122.03	110.80
1	A	113	ASP	N-CA-C	-5.27	99.58	110.80
2	B	290	THR	N-CA-C	-5.26	102.73	110.52
1	A	509	GLN	CA-C-N	5.25	126.41	119.84
1	A	509	GLN	C-N-CA	5.25	126.41	119.84
1	A	413	GLU	CB-CA-C	-5.22	103.38	109.80
2	B	298	GLU	N-CA-C	-5.21	106.31	113.56
2	B	132	ILE	CA-C-N	5.21	126.35	119.84
2	B	132	ILE	C-N-CA	5.21	126.35	119.84
1	A	143	ARG	N-CA-C	5.19	116.86	108.34
2	B	163	SER	N-CA-C	-5.19	105.53	111.14
1	A	51	GLY	N-CA-C	-5.19	101.76	112.34
1	A	420	PRO	N-CA-C	5.18	117.02	110.70
2	B	52	PRO	N-CA-C	5.17	123.13	112.47
1	A	408	ALA	N-CA-C	5.17	118.16	110.14
2	B	217	PRO	N-CA-C	-5.17	104.82	112.26
2	B	68	SER	N-CA-C	5.14	121.76	110.80
1	A	331	LYS	N-CA-C	-5.11	99.92	110.80
1	A	261	VAL	N-CA-C	-5.08	104.92	112.04
2	B	409	THR	N-CA-C	5.08	119.18	112.89
2	B	5	ILE	N-CA-C	-5.05	103.06	109.58
1	A	337	TRP	N-CA-C	5.03	117.26	108.76
1	A	416	PHE	N-CA-C	5.03	117.34	110.55
2	B	88	TRP	CA-CB-CG	5.01	123.11	113.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	183	TYR	Sidechain
2	B	188	TYR	Sidechain
2	B	354	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	56	TYR	Sidechain

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	4248	0	4052	583	4
2	B	3158	0	3082	392	1
3	A	20	0	14	3	0
All	All	7426	0	7148	947	4

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 65.

All (947) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:TYR:HE2	2:B:286:THR:HG23	1.19	1.07
2:B:150:PRO:HD2	2:B:153:TRP:HE1	1.17	1.06
1:A:42:GLU:HA	1:A:46:LYS:HA	1.36	1.05
1:A:79:GLU:HG2	1:A:83:ARG:HH21	1.23	1.01
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.36	1.00
2:B:206:ARG:HG2	2:B:217:PRO:HG2	1.43	1.00
1:A:542:ILE:HG23	1:A:545:ASN:HB3	1.43	0.99
2:B:278:GLN:HB3	2:B:298:GLU:HB3	1.43	0.97
1:A:447:ASN:HB2	1:A:556:ILE:HG23	1.47	0.96
1:A:84:THR:O	1:A:87:PHE:HB2	1.66	0.94
1:A:441:TYR:CE2	2:B:286:THR:HG23	2.03	0.94
2:B:223:LYS:O	2:B:225:PRO:HD3	1.67	0.94
1:A:50:ILE:HG22	1:A:52:PRO:HD3	1.50	0.91
1:A:188:TYR:O	3:A:557:NVP:HCB1	1.71	0.90
2:B:7:THR:HG21	2:B:122:GLU:HB2	1.53	0.90
2:B:282:LEU:HD11	2:B:293:ILE:HD11	1.54	0.89
1:A:419:THR:HG22	1:A:420:PRO:HD3	1.52	0.89
2:B:135:ILE:HD12	2:B:135:ILE:H	1.38	0.89
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.54	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:HA	1:A:281:LYS:HB2	1.56	0.88
1:A:170:PRO:HA	1:A:173:LYS:HE3	1.54	0.87
2:B:34:LEU:HD23	2:B:132:ILE:HG23	1.55	0.87
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.15	0.87
2:B:154:LYS:HD3	2:B:184:MET:SD	2.15	0.86
1:A:242:GLN:HB3	1:A:243:PRO:HD3	1.56	0.86
2:B:293:ILE:HB	2:B:294:PRO:HA	1.57	0.86
2:B:45:GLY:O	2:B:47:ILE:HG12	1.76	0.85
1:A:115:TYR:O	1:A:149:LEU:HB2	1.76	0.85
1:A:542:ILE:HD11	2:B:283:LEU:HD12	1.58	0.85
1:A:58:THR:HG21	1:A:77:PHE:HD2	1.42	0.85
2:B:254:VAL:HG23	2:B:283:LEU:HD22	1.57	0.85
1:A:34:LEU:HD13	1:A:62:ALA:HB2	1.57	0.84
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.59	0.84
2:B:44:GLU:HB3	2:B:47:ILE:HD11	1.57	0.84
2:B:194:GLU:HB2	2:B:197:GLN:O	1.77	0.84
2:B:376:THR:O	2:B:380:ILE:HD12	1.75	0.84
2:B:60:VAL:HG22	2:B:75:VAL:HG23	1.60	0.83
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.60	0.83
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.13	0.83
1:A:180:ILE:HG22	1:A:189:VAL:HA	1.61	0.83
2:B:34:LEU:HD13	2:B:62:ALA:HB2	1.59	0.83
1:A:103:LYS:HD2	1:A:191:SER:HA	1.60	0.83
1:A:386:THR:HG22	1:A:387:PRO:HD2	1.61	0.83
1:A:59:PRO:O	1:A:75:VAL:HG12	1.80	0.82
1:A:458:VAL:HG22	1:A:464:GLN:HB3	1.61	0.82
1:A:34:LEU:HD23	1:A:60:VAL:HG12	1.61	0.82
2:B:277:ARG:HA	2:B:280:CYS:HB3	1.59	0.82
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.60	0.82
1:A:96:HIS:HD2	1:A:97:PRO:HD2	1.43	0.81
1:A:58:THR:HG21	1:A:77:PHE:CD2	2.14	0.81
1:A:536:VAL:CG2	1:A:542:ILE:HG12	2.09	0.81
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.62	0.81
2:B:150:PRO:HD2	2:B:153:TRP:NE1	1.95	0.81
1:A:517:LEU:O	1:A:521:ILE:HD13	1.82	0.80
2:B:254:VAL:HG11	2:B:288:ALA:HA	1.64	0.80
2:B:11:LYS:HE2	2:B:11:LYS:HA	1.64	0.80
1:A:536:VAL:HG23	2:B:258:GLN:HG3	1.63	0.79
1:A:170:PRO:HG2	1:A:208:HIS:HE1	1.47	0.79
2:B:5:ILE:O	2:B:6:GLU:HG3	1.83	0.79
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:VAL:HG12	2:B:293:ILE:HG12	1.64	0.79
2:B:65:LYS:HE3	2:B:72:ARG:CZ	2.13	0.78
1:A:229:TRP:HB3	1:A:232:TYR:HB2	1.65	0.78
1:A:166:LYS:HE3	1:A:166:LYS:HA	1.65	0.78
2:B:143:ARG:HB3	2:B:143:ARG:HH11	1.48	0.78
1:A:88:TRP:CE2	1:A:155:GLY:HA2	2.18	0.78
1:A:436:GLY:H	2:B:289:LEU:HD13	1.49	0.78
1:A:135:ILE:N	1:A:139:THR:HA	1.99	0.78
1:A:253:THR:HA	1:A:292:VAL:HA	1.63	0.78
2:B:119:PRO:C	2:B:120:LEU:HD13	2.09	0.78
1:A:546:GLU:O	1:A:549:ASP:HB3	1.83	0.77
1:A:378:GLU:O	1:A:382:ILE:HG12	1.83	0.77
1:A:247:PRO:HB2	1:A:252:TRP:HZ2	1.48	0.77
1:A:77:PHE:O	1:A:81:ASN:HB2	1.83	0.77
2:B:296:THR:HB	2:B:299:ALA:CB	2.15	0.77
1:A:184:MET:O	1:A:186:ASP:N	2.18	0.77
1:A:393:ILE:O	1:A:416:PHE:HB2	1.85	0.77
1:A:164:MET:HA	1:A:167:ILE:HD12	1.68	0.76
2:B:52:PRO:HD2	2:B:53:GLU:OE1	1.86	0.76
1:A:101:LYS:HG2	1:A:320:ASP:HB3	1.68	0.76
1:A:232:TYR:HB3	1:A:234:LEU:HD23	1.67	0.76
1:A:135:ILE:H	1:A:139:THR:HA	1.49	0.75
1:A:441:TYR:O	1:A:457:TYR:HA	1.85	0.75
2:B:31:ILE:O	2:B:35:VAL:HG23	1.87	0.75
2:B:147:ASN:N	2:B:147:ASN:HD22	1.85	0.75
1:A:164:MET:HG3	1:A:168:LEU:HD12	1.68	0.75
1:A:443:ASP:O	1:A:552:VAL:HG11	1.86	0.75
1:A:254:VAL:HG12	1:A:289:LEU:O	1.86	0.74
1:A:361:HIS:HB2	1:A:510:PRO:CB	2.17	0.74
2:B:13:LYS:HG2	2:B:14:PRO:N	2.01	0.74
2:B:7:THR:HG22	2:B:120:LEU:HD23	1.69	0.74
2:B:253:THR:O	2:B:256:ASP:HB2	1.88	0.74
2:B:74:LEU:CD2	2:B:411:ILE:HD11	2.18	0.73
2:B:197:GLN:OE1	2:B:197:GLN:HA	1.88	0.73
2:B:293:ILE:HG21	2:B:295:LEU:O	1.88	0.73
2:B:164:MET:SD	2:B:168:LEU:HD12	2.28	0.73
2:B:293:ILE:HB	2:B:294:PRO:CA	2.18	0.73
1:A:535:TRP:CZ2	1:A:537:PRO:HA	2.24	0.72
2:B:304:ALA:HA	2:B:307:ARG:HB3	1.70	0.72
1:A:258:GLN:NE2	1:A:283:LEU:HD21	2.04	0.72
1:A:87:PHE:O	2:B:55:PRO:HD3	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLN:HA	1:A:350:LYS:NZ	2.05	0.72
2:B:423:VAL:HG12	2:B:425:LEU:O	1.90	0.72
1:A:238:LYS:HB2	1:A:316:GLY:HA3	1.72	0.71
2:B:77:PHE:CE1	2:B:128:THR:HG22	2.24	0.71
2:B:219:LYS:HG2	2:B:220:LYS:N	2.03	0.71
1:A:124:PHE:O	1:A:126:LYS:HG2	1.90	0.71
1:A:165:THR:HG23	1:A:182:GLN:HE21	1.54	0.71
1:A:405:TYR:HE1	1:A:406:TRP:CZ3	2.08	0.71
1:A:483:TYR:HB2	1:A:521:ILE:HD11	1.72	0.71
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.70	0.71
1:A:480:GLN:HG2	1:A:517:LEU:HD23	1.71	0.71
2:B:10:VAL:HA	2:B:88:TRP:CZ3	2.26	0.71
1:A:536:VAL:HG21	1:A:542:ILE:HG12	1.71	0.71
2:B:11:LYS:HZ1	2:B:12:LEU:HD21	1.54	0.70
1:A:208:HIS:O	1:A:212:TRP:HD1	1.74	0.70
1:A:503:LEU:HD12	1:A:504:GLY:N	2.06	0.70
1:A:77:PHE:CZ	1:A:150:PRO:HB2	2.26	0.70
2:B:271:TYR:HB3	2:B:272:PRO:HD2	1.73	0.70
1:A:258:GLN:HE22	1:A:283:LEU:HD21	1.56	0.70
1:A:57:ASN:ND2	1:A:58:THR:H	1.89	0.70
1:A:131:THR:HA	1:A:143:ARG:HG3	1.74	0.70
1:A:389:PHE:HB3	1:A:391:LEU:HD13	1.72	0.70
1:A:363:ASN:H	1:A:363:ASN:ND2	1.87	0.70
1:A:372:VAL:HG11	1:A:411:ILE:CD1	2.22	0.70
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.74	0.70
2:B:10:VAL:HG22	2:B:88:TRP:CZ2	2.27	0.70
2:B:345:PRO:O	2:B:347:LYS:N	2.24	0.70
1:A:435:VAL:HG12	2:B:289:LEU:HB2	1.73	0.69
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.73	0.69
1:A:361:HIS:HB2	1:A:510:PRO:HB2	1.73	0.69
2:B:372:VAL:O	2:B:376:THR:HG22	1.91	0.69
2:B:376:THR:OG1	2:B:386:THR:HG22	1.92	0.69
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.26	0.69
2:B:45:GLY:O	2:B:47:ILE:N	2.25	0.69
1:A:247:PRO:HB2	1:A:252:TRP:CZ2	2.27	0.69
2:B:47:ILE:HG22	2:B:148:VAL:HG21	1.75	0.69
1:A:64:LYS:CB	1:A:72:ARG:H	2.06	0.69
1:A:56:TYR:O	1:A:57:ASN:HB2	1.93	0.69
1:A:245:VAL:HG22	1:A:247:PRO:HD3	1.73	0.69
1:A:193:LEU:HD22	1:A:197:GLN:HE21	1.58	0.69
1:A:235:HIS:HD2	1:A:237:ASP:HB2	1.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:HE2	1:A:457:TYR:CZ	2.11	0.68
1:A:165:THR:HG23	1:A:182:GLN:NE2	2.09	0.68
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.75	0.68
2:B:65:LYS:HA	2:B:407:GLN:HG2	1.75	0.68
2:B:48:SER:HA	2:B:145:GLN:O	1.93	0.67
2:B:57:ASN:ND2	2:B:143:ARG:HH12	1.91	0.67
1:A:435:VAL:HG12	2:B:289:LEU:CB	2.24	0.67
2:B:11:LYS:NZ	2:B:12:LEU:HD21	2.08	0.67
2:B:369:THR:HG22	2:B:370:GLU:HG3	1.76	0.67
1:A:433:PRO:HB3	1:A:532:TYR:CE2	2.29	0.67
1:A:178:ILE:O	1:A:178:ILE:HD13	1.94	0.66
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.30	0.66
1:A:513:SER:HB2	1:A:519:ASN:ND2	2.11	0.66
1:A:242:GLN:O	1:A:244:ILE:HG13	1.95	0.66
2:B:65:LYS:HG3	2:B:72:ARG:HD3	1.77	0.66
1:A:361:HIS:CG	1:A:511:ASP:O	2.49	0.66
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.76	0.66
1:A:124:PHE:O	1:A:126:LYS:N	2.29	0.66
1:A:261:VAL:HG11	1:A:280:CYS:HB3	1.77	0.66
2:B:282:LEU:HG	2:B:292:VAL:HG11	1.78	0.66
1:A:57:ASN:OD1	1:A:131:THR:HG22	1.95	0.65
1:A:164:MET:O	1:A:168:LEU:HD12	1.97	0.65
1:A:529:GLU:O	1:A:529:GLU:HG2	1.95	0.65
1:A:536:VAL:HG22	1:A:542:ILE:HG12	1.77	0.65
2:B:74:LEU:HD21	2:B:411:ILE:HD11	1.78	0.65
1:A:101:LYS:CG	1:A:320:ASP:HB3	2.26	0.65
2:B:286:THR:HG22	2:B:287:LYS:N	2.11	0.65
2:B:321:PRO:O	2:B:323:LYS:N	2.30	0.65
1:A:13:LYS:NZ	1:A:82:LYS:O	2.29	0.65
1:A:416:PHE:CD1	1:A:417:VAL:N	2.65	0.65
2:B:65:LYS:HG3	2:B:72:ARG:CD	2.27	0.65
2:B:118:VAL:HB	2:B:119:PRO:HD3	1.78	0.65
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.27	0.65
1:A:542:ILE:CD1	2:B:283:LEU:HD12	2.27	0.64
1:A:229:TRP:HA	1:A:229:TRP:HE3	1.63	0.64
1:A:33:ALA:HB2	1:A:71:TRP:HE3	1.62	0.64
1:A:242:GLN:CB	1:A:243:PRO:HD3	2.28	0.64
1:A:542:ILE:HG23	1:A:545:ASN:CB	2.25	0.64
2:B:198:HIS:O	2:B:202:ILE:HG12	1.98	0.64
1:A:457:TYR:CD1	1:A:457:TYR:C	2.75	0.64
1:A:77:PHE:HZ	1:A:150:PRO:HB2	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:O	1:A:357:MET:SD	2.56	0.64
1:A:79:GLU:CG	1:A:83:ARG:HH21	2.05	0.64
2:B:28:GLU:HA	2:B:31:ILE:HG23	1.79	0.64
1:A:41:MET:HB3	1:A:48:SER:OG	1.97	0.64
2:B:200:THR:HG23	2:B:201:LYS:H	1.61	0.64
2:B:305:GLU:O	2:B:309:ILE:HG12	1.98	0.64
1:A:195:ILE:O	1:A:199:ARG:HG2	1.98	0.64
1:A:301:LEU:HA	1:A:304:ALA:HB3	1.79	0.63
1:A:391:LEU:O	1:A:416:PHE:HA	1.96	0.63
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.80	0.63
2:B:195:ILE:C	2:B:197:GLN:H	2.07	0.63
2:B:277:ARG:CA	2:B:280:CYS:HB3	2.27	0.63
1:A:32:LYS:O	1:A:36:GLU:HG2	1.97	0.63
1:A:539:HIS:O	1:A:542:ILE:HG22	1.98	0.63
2:B:332:GLN:HA	2:B:337:TRP:CD1	2.34	0.63
2:B:395:LYS:O	2:B:396:GLU:HB2	1.97	0.63
2:B:12:LEU:HD23	2:B:12:LEU:N	2.13	0.63
1:A:34:LEU:HD11	1:A:73:LYS:HB2	1.81	0.63
2:B:304:ALA:HA	2:B:307:ARG:CB	2.29	0.63
2:B:366:LYS:HZ2	2:B:405:TYR:HB3	1.64	0.63
2:B:39:THR:O	2:B:43:LYS:HG2	1.98	0.63
2:B:43:LYS:C	2:B:45:GLY:H	2.05	0.63
2:B:296:THR:HB	2:B:299:ALA:HB3	1.79	0.63
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.34	0.62
1:A:132:ILE:HB	1:A:142:ILE:HB	1.81	0.62
2:B:280:CYS:SG	2:B:281:LYS:N	2.72	0.62
1:A:12:LEU:HA	1:A:84:THR:CG2	2.29	0.62
1:A:539:HIS:CG	1:A:540:LYS:N	2.68	0.62
2:B:368:LEU:HD23	2:B:393:ILE:HD12	1.81	0.62
1:A:131:THR:HB	1:A:143:ARG:HD2	1.81	0.62
1:A:175:ASN:OD1	1:A:175:ASN:N	2.32	0.62
1:A:245:VAL:HG22	1:A:246:LEU:H	1.65	0.62
1:A:95:PRO:HA	2:B:136:ASN:OD1	1.99	0.62
2:B:108:VAL:HA	2:B:187:LEU:O	1.98	0.62
1:A:52:PRO:HA	1:A:143:ARG:HB3	1.81	0.62
2:B:116:PHE:O	2:B:119:PRO:HD2	1.98	0.62
1:A:42:GLU:CA	1:A:46:LYS:HA	2.21	0.62
1:A:165:THR:O	1:A:169:GLU:HG2	2.00	0.62
2:B:220:LYS:HB2	2:B:222:GLN:NE2	2.15	0.62
1:A:88:TRP:NE1	1:A:155:GLY:HA2	2.15	0.62
1:A:239:TRP:HH2	1:A:349:LEU:O	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG11	1:A:288:ALA:O	2.00	0.61
2:B:140:PRO:HG2	2:B:142:ILE:HD11	1.81	0.61
1:A:79:GLU:HG2	1:A:83:ARG:NH2	2.06	0.61
1:A:439:THR:HG21	2:B:288:ALA:H	1.64	0.61
1:A:501:TYR:HD1	1:A:502:ALA:N	1.99	0.61
2:B:125:ARG:HB3	2:B:146:TYR:O	2.00	0.61
2:B:286:THR:HG22	2:B:287:LYS:H	1.64	0.61
1:A:317:VAL:CB	1:A:349:LEU:HA	2.30	0.61
1:A:361:HIS:CE1	1:A:512:LYS:O	2.53	0.61
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.32	0.61
1:A:239:TRP:HZ3	1:A:317:VAL:CB	2.14	0.61
1:A:456:GLY:O	1:A:457:TYR:HB3	2.00	0.61
1:A:77:PHE:N	1:A:77:PHE:CD1	2.66	0.61
1:A:164:MET:HG3	1:A:164:MET:O	2.00	0.61
2:B:354:TYR:HB2	2:B:374:LYS:HD2	1.82	0.61
2:B:3:SER:HB3	2:B:4:PRO:O	2.00	0.60
1:A:12:LEU:O	1:A:13:LYS:C	2.43	0.60
1:A:171:PHE:C	1:A:173:LYS:H	2.08	0.60
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.37	0.60
1:A:258:GLN:NE2	1:A:283:LEU:HD11	2.16	0.60
1:A:296:THR:HG23	1:A:297:GLU:N	2.16	0.60
1:A:434:ILE:HG21	1:A:492:GLU:CG	2.31	0.60
1:A:52:PRO:CB	1:A:143:ARG:HB2	2.31	0.60
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.83	0.60
1:A:434:ILE:HD13	1:A:492:GLU:HG3	1.83	0.60
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.83	0.60
2:B:91:GLN:O	2:B:92:LEU:HB2	2.02	0.60
1:A:234:LEU:HB3	1:A:239:TRP:HB2	1.82	0.60
2:B:257:ILE:HA	2:B:260:LEU:HB3	1.82	0.60
1:A:443:ASP:HB2	1:A:548:VAL:HG13	1.84	0.60
2:B:123:ASP:H	2:B:125:ARG:NE	2.00	0.60
2:B:253:THR:HA	2:B:291:GLU:HA	1.84	0.60
1:A:19:PRO:HB3	1:A:79:GLU:HB3	1.82	0.60
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.83	0.60
2:B:252:TRP:CZ2	2:B:260:LEU:HD22	2.37	0.60
2:B:65:LYS:HE3	2:B:72:ARG:NE	2.17	0.59
1:A:144:TYR:O	1:A:145:GLN:HB3	2.01	0.59
1:A:171:PHE:O	1:A:173:LYS:N	2.34	0.59
1:A:12:LEU:HG	1:A:83:ARG:O	2.03	0.59
1:A:235:HIS:CD2	1:A:237:ASP:HB2	2.35	0.59
1:A:300:GLU:O	1:A:304:ALA:HB2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:HA	1:A:281:LYS:CB	2.31	0.59
2:B:39:THR:HG23	2:B:40:GLU:OE2	2.01	0.59
2:B:86:ASP:O	2:B:89:GLU:HB3	2.02	0.59
2:B:296:THR:HB	2:B:299:ALA:HB2	1.82	0.59
1:A:12:LEU:HA	1:A:84:THR:HG23	1.84	0.59
1:A:114:ALA:C	1:A:116:PHE:H	2.09	0.59
2:B:128:THR:HG21	2:B:150:PRO:HG2	1.85	0.59
1:A:183:TYR:C	1:A:184:MET:HG2	2.28	0.59
2:B:65:LYS:HD3	2:B:407:GLN:O	2.03	0.59
1:A:52:PRO:HB3	1:A:143:ARG:HB2	1.85	0.58
1:A:398:TRP:CE3	1:A:402:TRP:CD1	2.91	0.58
2:B:2:ILE:HD12	2:B:2:ILE:O	2.02	0.58
1:A:57:ASN:HD22	1:A:58:THR:H	1.48	0.58
2:B:266:TRP:HZ3	2:B:422:LEU:CD2	2.16	0.58
2:B:276:VAL:O	2:B:279:LEU:HB3	2.03	0.58
1:A:11:LYS:N	1:A:87:PHE:HE2	2.00	0.58
1:A:183:TYR:O	1:A:184:MET:HG2	2.03	0.58
2:B:417:VAL:O	2:B:417:VAL:HG13	2.03	0.58
1:A:210:LEU:HD23	1:A:210:LEU:O	2.03	0.58
1:A:176:PRO:O	1:A:177:ASP:HB2	2.03	0.58
1:A:271:TYR:O	1:A:274:ILE:HG12	2.04	0.58
2:B:219:LYS:HG2	2:B:220:LYS:H	1.67	0.58
1:A:31:ILE:HD11	1:A:133:PRO:HD2	1.86	0.58
1:A:8:VAL:O	1:A:10:VAL:HG13	2.05	0.57
2:B:40:GLU:O	2:B:44:GLU:HB2	2.04	0.57
1:A:31:ILE:O	1:A:35:VAL:HG23	2.04	0.57
1:A:362:THR:HG22	1:A:366:LYS:HB3	1.84	0.57
2:B:66:LYS:H	2:B:407:GLN:NE2	2.02	0.57
2:B:364:ASP:HA	2:B:367:GLN:HB2	1.85	0.57
1:A:10:VAL:HG12	1:A:88:TRP:CH2	2.39	0.57
2:B:378:GLU:O	2:B:382:ILE:HG13	2.05	0.57
1:A:69:THR:O	1:A:69:THR:HG22	2.04	0.57
1:A:465:LYS:HG2	1:A:466:VAL:N	2.18	0.57
1:A:461:LYS:O	1:A:463:ARG:N	2.37	0.57
2:B:146:TYR:C	2:B:147:ASN:HD22	2.12	0.57
2:B:425:LEU:O	2:B:426:TRP:HB3	2.05	0.57
1:A:167:ILE:HD13	1:A:214:LEU:HD11	1.85	0.57
1:A:366:LYS:O	1:A:370:GLU:HG3	2.05	0.57
2:B:260:LEU:HD21	2:B:279:LEU:HD11	1.84	0.57
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.40	0.57
1:A:296:THR:HG22	1:A:299:ALA:H	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:CH2	1:A:411:ILE:HG21	2.40	0.57
2:B:263:LYS:HG3	2:B:425:LEU:HB3	1.86	0.57
1:A:424:LYS:C	1:A:426:TRP:H	2.13	0.57
1:A:535:TRP:CH2	1:A:537:PRO:HA	2.40	0.57
2:B:270:ILE:O	2:B:271:TYR:CG	2.57	0.57
1:A:5:ILE:HG22	1:A:6:GLU:N	2.20	0.57
1:A:35:VAL:C	1:A:37:ILE:H	2.11	0.57
1:A:183:TYR:HE2	1:A:230:MET:HE2	1.70	0.57
1:A:95:PRO:HG2	1:A:181:TYR:CE2	2.40	0.57
1:A:203:GLU:HG2	1:A:206:ARG:HH22	1.70	0.57
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.86	0.57
2:B:183:TYR:CE2	2:B:380:ILE:HG12	2.39	0.57
2:B:278:GLN:HB3	2:B:298:GLU:CB	2.26	0.57
2:B:397:THR:HG22	2:B:397:THR:O	2.04	0.57
2:B:194:GLU:O	2:B:197:GLN:N	2.38	0.56
1:A:180:ILE:CG2	1:A:189:VAL:HG13	2.36	0.56
1:A:184:MET:O	1:A:185:ASP:C	2.48	0.56
1:A:362:THR:CG2	1:A:366:LYS:HG3	2.35	0.56
1:A:506:ILE:HD13	1:A:506:ILE:N	2.21	0.56
2:B:143:ARG:HH11	2:B:143:ARG:CB	2.17	0.56
1:A:35:VAL:C	1:A:37:ILE:N	2.61	0.56
1:A:47:ILE:HG22	1:A:47:ILE:O	2.05	0.56
1:A:75:VAL:HG23	1:A:75:VAL:O	2.05	0.56
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.41	0.56
2:B:389:PHE:O	2:B:415:GLU:N	2.37	0.56
1:A:79:GLU:O	1:A:83:ARG:HG2	2.06	0.56
1:A:276:VAL:HG12	1:A:280:CYS:SG	2.45	0.56
2:B:115:TYR:HE2	2:B:185:ASP:HA	1.70	0.56
2:B:163:SER:O	2:B:167:ILE:HG13	2.05	0.56
1:A:52:PRO:O	1:A:143:ARG:NH1	2.37	0.56
2:B:253:THR:HG22	2:B:256:ASP:H	1.68	0.56
1:A:5:ILE:HG22	1:A:6:GLU:H	1.71	0.56
1:A:116:PHE:O	1:A:148:VAL:HG11	2.05	0.56
2:B:7:THR:HG21	2:B:122:GLU:CB	2.32	0.56
2:B:116:PHE:O	2:B:118:VAL:N	2.39	0.56
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.88	0.56
1:A:483:TYR:HE1	1:A:524:GLN:HE22	1.53	0.56
2:B:282:LEU:HG	2:B:292:VAL:CG1	2.36	0.56
2:B:366:LYS:HA	2:B:366:LYS:HZ3	1.70	0.56
1:A:122:GLU:HG3	1:A:125:ARG:NH1	2.21	0.56
2:B:191:SER:OG	2:B:198:HIS:HD2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:PRO:O	2:B:141:GLY:C	2.48	0.55
2:B:267:ALA:O	2:B:269:GLN:N	2.40	0.55
1:A:52:PRO:HA	1:A:143:ARG:CB	2.36	0.55
1:A:194:GLU:O	1:A:195:ILE:C	2.50	0.55
1:A:398:TRP:CZ3	1:A:402:TRP:CD1	2.94	0.55
2:B:34:LEU:CD1	2:B:62:ALA:HB2	2.33	0.55
2:B:424:LYS:O	2:B:425:LEU:HB2	2.04	0.55
1:A:42:GLU:HA	1:A:46:LYS:CA	2.23	0.55
1:A:56:TYR:N	1:A:56:TYR:CD1	2.74	0.55
1:A:341:ILE:HD11	1:A:375:ILE:HG23	1.87	0.55
1:A:168:LEU:HD22	1:A:180:ILE:HD11	1.89	0.55
1:A:501:TYR:CD1	1:A:502:ALA:N	2.75	0.55
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.30	0.55
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.06	0.55
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.87	0.55
1:A:363:ASN:ND2	1:A:363:ASN:N	2.54	0.55
2:B:280:CYS:O	2:B:282:LEU:N	2.40	0.55
1:A:491:LEU:HB3	1:A:529:GLU:OE2	2.06	0.55
1:A:34:LEU:CD1	1:A:62:ALA:HB2	2.34	0.54
2:B:304:ALA:O	2:B:307:ARG:HB3	2.07	0.54
2:B:425:LEU:O	2:B:426:TRP:CB	2.54	0.54
1:A:74:LEU:HD12	1:A:75:VAL:N	2.22	0.54
1:A:193:LEU:HB2	1:A:198:HIS:CD2	2.42	0.54
1:A:441:TYR:CZ	1:A:544:GLY:HA3	2.42	0.54
1:A:10:VAL:HG12	1:A:88:TRP:HH2	1.72	0.54
1:A:56:TYR:O	1:A:143:ARG:NH2	2.41	0.54
2:B:46:LYS:HB3	2:B:148:VAL:HG13	1.89	0.54
2:B:300:GLU:OE1	2:B:303:LEU:HD22	2.08	0.54
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.43	0.54
1:A:168:LEU:O	1:A:172:LYS:HB2	2.07	0.54
1:A:473:THR:HB	1:A:476:LYS:HE3	1.90	0.54
2:B:292:VAL:CG1	2:B:293:ILE:HG12	2.37	0.54
1:A:164:MET:CE	1:A:214:LEU:HD13	2.37	0.54
2:B:39:THR:HG23	2:B:40:GLU:N	2.22	0.54
2:B:332:GLN:HA	2:B:337:TRP:NE1	2.23	0.54
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.38	0.54
1:A:326:ILE:H	1:A:343:GLN:NE2	2.06	0.54
1:A:411:ILE:O	1:A:411:ILE:HG23	2.08	0.54
2:B:41:MET:O	2:B:47:ILE:HG13	2.07	0.54
2:B:192:ASP:O	2:B:194:GLU:N	2.41	0.54
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG13	1:A:108:VAL:O	2.07	0.53
1:A:280:CYS:O	1:A:283:LEU:HB3	2.08	0.53
2:B:85:GLN:OE1	2:B:89:GLU:HB2	2.08	0.53
2:B:100:LEU:O	2:B:100:LEU:HD12	2.08	0.53
1:A:53:GLU:O	1:A:54:ASN:HB2	2.08	0.53
1:A:58:THR:HG23	1:A:59:PRO:CD	2.38	0.53
1:A:193:LEU:HD22	1:A:197:GLN:HG3	1.90	0.53
1:A:232:TYR:HA	1:A:240:THR:O	2.08	0.53
2:B:270:ILE:O	2:B:271:TYR:CD1	2.61	0.53
2:B:206:ARG:CZ	2:B:219:LYS:H	2.22	0.53
1:A:254:VAL:O	1:A:258:GLN:HG2	2.08	0.53
1:A:271:TYR:HB3	1:A:274:ILE:HD11	1.90	0.53
1:A:405:TYR:HE1	1:A:406:TRP:CE3	2.27	0.53
1:A:503:LEU:HD13	1:A:507:GLN:OE1	2.08	0.53
2:B:254:VAL:HG12	2:B:290:THR:O	2.09	0.53
1:A:104:LYS:CB	1:A:192:ASP:HA	2.38	0.53
1:A:131:THR:HB	1:A:143:ARG:CD	2.39	0.53
1:A:135:ILE:H	1:A:140:PRO:HD2	1.74	0.53
1:A:208:HIS:CD2	1:A:212:TRP:HE1	2.27	0.53
1:A:224:GLU:OE2	1:A:226:PRO:HD2	2.09	0.53
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.38	0.53
1:A:457:TYR:C	1:A:457:TYR:HD1	2.15	0.53
2:B:4:PRO:HG2	2:B:5:ILE:H	1.73	0.53
1:A:282:LEU:HD12	1:A:282:LEU:H	1.73	0.53
2:B:173:LYS:HD3	2:B:173:LYS:C	2.33	0.53
1:A:321:PRO:HG2	1:A:343:GLN:HG2	1.89	0.52
1:A:443:ASP:C	1:A:552:VAL:HG11	2.33	0.52
2:B:178:ILE:HG22	2:B:178:ILE:O	2.09	0.52
2:B:354:TYR:OH	2:B:367:GLN:HG3	2.08	0.52
1:A:10:VAL:HG22	1:A:121:ASP:OD2	2.09	0.52
2:B:366:LYS:HE3	2:B:404:GLU:HB2	1.91	0.52
1:A:10:VAL:HG23	1:A:10:VAL:O	2.08	0.52
1:A:441:TYR:CE1	1:A:544:GLY:HA3	2.44	0.52
2:B:380:ILE:O	2:B:381:VAL:C	2.53	0.52
1:A:10:VAL:CG1	1:A:88:TRP:HH2	2.22	0.52
1:A:282:LEU:O	1:A:284:ARG:N	2.42	0.52
1:A:411:ILE:HG13	1:A:412:PRO:HD2	1.91	0.52
2:B:46:LYS:HZ3	2:B:117:SER:HA	1.73	0.52
2:B:47:ILE:CG2	2:B:148:VAL:HG21	2.39	0.52
2:B:129:ALA:O	2:B:130:PHE:HB3	2.10	0.52
2:B:252:TRP:HB2	2:B:294:PRO:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:CB	1:A:71:TRP:HE3	2.22	0.52
2:B:115:TYR:CE2	2:B:185:ASP:HA	2.45	0.52
2:B:115:TYR:O	2:B:149:LEU:HB2	2.09	0.52
2:B:285:GLY:O	2:B:286:THR:OG1	2.25	0.52
1:A:10:VAL:HA	1:A:87:PHE:CE2	2.45	0.52
1:A:42:GLU:C	1:A:46:LYS:HG2	2.35	0.52
1:A:200:THR:O	1:A:203:GLU:HB2	2.10	0.52
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.43	0.52
2:B:88:TRP:CE2	2:B:92:LEU:HD13	2.45	0.52
2:B:366:LYS:NZ	2:B:369:THR:HG21	2.25	0.52
1:A:203:GLU:HA	1:A:206:ARG:NH1	2.25	0.52
1:A:419:THR:CG2	1:A:420:PRO:HD3	2.34	0.52
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.35	0.51
1:A:210:LEU:HG	1:A:215:THR:HA	1.93	0.51
1:A:444:GLY:HA2	1:A:454:LYS:O	2.10	0.51
1:A:120:LEU:O	1:A:121:ASP:O	2.27	0.51
1:A:178:ILE:HA	1:A:191:SER:HB3	1.92	0.51
1:A:235:HIS:HD2	1:A:237:ASP:CB	2.22	0.51
1:A:239:TRP:O	1:A:316:GLY:N	2.43	0.51
1:A:517:LEU:C	1:A:521:ILE:HD13	2.36	0.51
2:B:77:PHE:CZ	2:B:128:THR:HG22	2.45	0.51
1:A:35:VAL:O	1:A:37:ILE:N	2.43	0.51
1:A:405:TYR:CE2	1:A:407:GLN:HG2	2.45	0.51
2:B:218:ASP:O	2:B:221:HIS:CE1	2.64	0.51
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.45	0.51
1:A:372:VAL:HG21	1:A:411:ILE:HD11	1.92	0.51
1:A:167:ILE:CD1	1:A:214:LEU:HD11	2.39	0.51
1:A:537:PRO:CG	2:B:262:GLY:HA2	2.40	0.51
1:A:97:PRO:O	1:A:99:GLY:N	2.44	0.51
1:A:282:LEU:HD12	1:A:282:LEU:N	2.26	0.51
1:A:287:LYS:O	1:A:288:ALA:HB2	2.10	0.51
1:A:394:GLN:O	1:A:395:LYS:C	2.53	0.51
2:B:135:ILE:H	2:B:135:ILE:CD1	2.16	0.51
2:B:302:GLU:HA	2:B:305:GLU:HB3	1.92	0.51
1:A:342:TYR:HA	1:A:349:LEU:HB2	1.93	0.51
2:B:10:VAL:O	2:B:11:LYS:HE2	2.10	0.51
2:B:33:ALA:O	2:B:36:GLU:N	2.42	0.51
2:B:312:GLU:HB3	2:B:313:PRO:CD	2.39	0.51
1:A:80:LEU:HD22	1:A:153:TRP:HE1	1.75	0.50
2:B:93:GLY:O	2:B:95:PRO:HD3	2.11	0.50
2:B:261:VAL:HG12	2:B:262:GLY:N	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLU:HG2	2:B:40:GLU:OE1	2.10	0.50
1:A:166:LYS:HE3	1:A:166:LYS:CA	2.38	0.50
1:A:312:GLU:C	1:A:314:VAL:H	2.19	0.50
1:A:403:THR:HG22	1:A:404:GLU:HG3	1.93	0.50
2:B:43:LYS:C	2:B:45:GLY:N	2.70	0.50
2:B:257:ILE:HG23	2:B:261:VAL:HG23	1.93	0.50
1:A:284:ARG:O	1:A:286:THR:N	2.44	0.50
1:A:379:SER:HA	1:A:383:TRP:CZ3	2.47	0.50
1:A:421:PRO:C	1:A:423:VAL:H	2.19	0.50
1:A:460:ASN:HB2	2:B:287:LYS:HG2	1.93	0.50
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.58	0.50
2:B:257:ILE:O	2:B:261:VAL:HB	2.12	0.50
1:A:103:LYS:HD2	1:A:190:GLY:O	2.11	0.50
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.92	0.50
2:B:377:THR:HG1	2:B:410:TRP:HZ2	1.58	0.50
1:A:372:VAL:HG11	1:A:411:ILE:CG1	2.42	0.50
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.76	0.50
1:A:29:GLU:C	1:A:71:TRP:HZ3	2.20	0.50
1:A:166:LYS:HA	1:A:166:LYS:CE	2.40	0.50
1:A:406:TRP:CD1	1:A:406:TRP:C	2.90	0.50
2:B:271:TYR:HB3	2:B:272:PRO:CD	2.39	0.50
1:A:108:VAL:HG21	1:A:188:TYR:CZ	2.46	0.50
1:A:261:VAL:HB	1:A:276:VAL:HG11	1.93	0.50
2:B:263:LYS:HG3	2:B:425:LEU:CB	2.42	0.50
1:A:193:LEU:HB2	1:A:198:HIS:HD2	1.76	0.49
2:B:366:LYS:NZ	2:B:405:TYR:H	2.10	0.49
1:A:38:CYS:O	1:A:41:MET:HB2	2.12	0.49
1:A:48:SER:HA	1:A:147:ASN:OD1	2.11	0.49
1:A:134:SER:CB	1:A:141:GLY:H	2.25	0.49
1:A:269:GLN:HA	1:A:350:LYS:HZ2	1.77	0.49
1:A:505:ILE:O	1:A:510:PRO:HD3	2.11	0.49
2:B:79:GLU:OE1	2:B:82:LYS:HE2	2.13	0.49
1:A:34:LEU:HD13	1:A:62:ALA:CB	2.36	0.49
1:A:539:HIS:CG	1:A:540:LYS:H	2.30	0.49
1:A:548:VAL:O	1:A:549:ASP:C	2.53	0.49
2:B:266:TRP:HZ3	2:B:422:LEU:HD23	1.77	0.49
1:A:170:PRO:C	1:A:174:GLN:HE21	2.20	0.49
2:B:259:LYS:O	2:B:260:LEU:C	2.56	0.49
1:A:406:TRP:CD1	2:B:421:PRO:HD3	2.48	0.49
2:B:297:GLU:O	2:B:298:GLU:HB2	2.12	0.49
1:A:484:LEU:O	1:A:487:GLN:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PHE:CE2	2:B:402:TRP:CZ2	3.00	0.49
2:B:80:LEU:O	2:B:84:THR:N	2.42	0.49
2:B:175:ASN:HD21	2:B:201:LYS:HE2	1.78	0.49
1:A:239:TRP:CD1	1:A:240:THR:N	2.80	0.49
1:A:361:HIS:NE2	1:A:512:LYS:O	2.46	0.49
2:B:46:LYS:O	2:B:48:SER:N	2.46	0.49
1:A:328:GLU:CB	1:A:341:ILE:HD12	2.42	0.49
1:A:386:THR:CG2	1:A:387:PRO:HD2	2.40	0.49
2:B:193:LEU:HD13	2:B:193:LEU:N	2.27	0.49
2:B:293:ILE:HG21	2:B:295:LEU:C	2.38	0.49
1:A:110:ASP:O	1:A:216:THR:HG22	2.12	0.49
1:A:406:TRP:CE2	2:B:420:PRO:HB3	2.47	0.49
2:B:36:GLU:O	2:B:39:THR:HG22	2.11	0.49
2:B:270:ILE:HG12	2:B:346:PHE:CB	2.42	0.49
1:A:361:HIS:HB2	1:A:510:PRO:HB3	1.95	0.49
1:A:362:THR:HG22	1:A:366:LYS:HG3	1.94	0.49
2:B:61:PHE:CE2	2:B:402:TRP:HZ2	2.30	0.49
2:B:366:LYS:HZ2	2:B:405:TYR:CB	2.26	0.49
1:A:31:ILE:CD1	1:A:133:PRO:HD2	2.43	0.48
2:B:390:LYS:HB3	2:B:417:VAL:HG11	1.95	0.48
1:A:40:GLU:C	1:A:42:GLU:H	2.20	0.48
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.94	0.48
1:A:543:GLY:HA3	2:B:283:LEU:O	2.13	0.48
2:B:3:SER:HB3	2:B:4:PRO:CA	2.42	0.48
2:B:193:LEU:HD22	2:B:193:LEU:H	1.79	0.48
1:A:543:GLY:CA	2:B:283:LEU:O	2.62	0.48
2:B:22:LYS:O	2:B:23:GLN:HB2	2.12	0.48
2:B:427:TYR:HD1	2:B:427:TYR:H	1.60	0.48
1:A:112:GLY:O	1:A:114:ALA:N	2.46	0.48
1:A:398:TRP:O	1:A:399:GLU:C	2.55	0.48
1:A:537:PRO:HG2	2:B:262:GLY:HA2	1.93	0.48
2:B:85:GLN:O	2:B:86:ASP:C	2.53	0.48
2:B:197:GLN:O	2:B:198:HIS:HB2	2.14	0.48
2:B:214:LEU:O	2:B:215:THR:C	2.56	0.48
1:A:34:LEU:HD11	1:A:73:LYS:CB	2.44	0.48
1:A:372:VAL:HG11	1:A:411:ILE:HD11	1.94	0.48
1:A:391:LEU:HD22	1:A:414:TRP:HB2	1.96	0.48
2:B:254:VAL:HG13	2:B:255:ASN:H	1.78	0.48
1:A:171:PHE:C	1:A:173:LYS:N	2.72	0.48
1:A:276:VAL:O	1:A:276:VAL:CG1	2.61	0.48
1:A:357:MET:SD	1:A:357:MET:C	2.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:O	1:A:367:GLN:N	2.43	0.48
1:A:440:PHE:CE2	1:A:457:TYR:CE1	3.01	0.48
2:B:153:TRP:CZ3	2:B:155:GLY:HA3	2.48	0.48
2:B:304:ALA:O	2:B:307:ARG:N	2.46	0.48
1:A:107:THR:N	1:A:189:VAL:O	2.47	0.48
1:A:528:LYS:O	1:A:529:GLU:C	2.57	0.48
1:A:405:TYR:CE1	1:A:406:TRP:CE3	3.01	0.48
2:B:81:ASN:O	2:B:82:LYS:C	2.55	0.48
2:B:277:ARG:O	2:B:280:CYS:HB3	2.13	0.48
2:B:306:ASN:O	2:B:309:ILE:HB	2.14	0.48
2:B:380:ILE:HD11	2:B:386:THR:CG2	2.43	0.48
1:A:458:VAL:HG22	1:A:464:GLN:CB	2.39	0.48
1:A:108:VAL:HA	1:A:187:LEU:O	2.14	0.48
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.96	0.48
1:A:546:GLU:O	1:A:550:LYS:HG2	2.13	0.48
2:B:63:ILE:CD1	2:B:74:LEU:HD12	2.44	0.48
1:A:79:GLU:O	1:A:80:LEU:C	2.57	0.47
1:A:103:LYS:CD	1:A:191:SER:HA	2.40	0.47
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.48	0.47
1:A:536:VAL:CG2	2:B:258:GLN:HE21	2.28	0.47
1:A:536:VAL:HG21	2:B:258:GLN:HE21	1.79	0.47
2:B:47:ILE:HG22	2:B:148:VAL:CG2	2.44	0.47
2:B:99:GLY:O	2:B:102:LYS:N	2.47	0.47
2:B:46:LYS:NZ	2:B:117:SER:HA	2.29	0.47
2:B:284:ARG:H	2:B:284:ARG:HD2	1.79	0.47
1:A:298:GLU:O	1:A:301:LEU:N	2.45	0.47
2:B:188:TYR:OH	2:B:410:TRP:CZ3	2.67	0.47
1:A:13:LYS:HG3	1:A:84:THR:N	2.29	0.47
1:A:77:PHE:HZ	1:A:150:PRO:CB	2.28	0.47
1:A:209:LEU:O	1:A:211:ARG:N	2.47	0.47
1:A:537:PRO:O	1:A:539:HIS:N	2.48	0.47
1:A:3:SER:OG	1:A:5:ILE:HG13	2.15	0.47
1:A:114:ALA:O	1:A:116:PHE:N	2.48	0.47
1:A:483:TYR:HE1	1:A:524:GLN:NE2	2.13	0.47
1:A:498:ASP:HA	1:A:536:VAL:O	2.15	0.47
2:B:21:VAL:HG12	2:B:22:LYS:H	1.80	0.47
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.33	0.47
2:B:354:TYR:O	2:B:355:ALA:HB2	2.15	0.47
1:A:42:GLU:O	1:A:46:LYS:HG2	2.14	0.47
1:A:318:TYR:HD1	1:A:318:TYR:O	1.97	0.47
1:A:354:TYR:HD2	1:A:371:ALA:HB2	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:C	1:A:426:TRP:N	2.72	0.47
1:A:502:ALA:O	1:A:506:ILE:HG12	2.14	0.47
2:B:84:THR:OG1	2:B:85:GLN:N	2.48	0.47
2:B:92:LEU:O	2:B:161:GLN:NE2	2.48	0.47
2:B:302:GLU:HA	2:B:305:GLU:CB	2.45	0.47
1:A:34:LEU:CD2	1:A:60:VAL:HG12	2.39	0.47
1:A:401:TRP:O	1:A:405:TYR:N	2.47	0.47
1:A:506:ILE:HD13	1:A:506:ILE:H	1.79	0.47
2:B:63:ILE:HD11	2:B:74:LEU:HD12	1.97	0.47
1:A:51:GLY:N	1:A:52:PRO:CD	2.78	0.47
1:A:160:PHE:C	1:A:162:SER:N	2.69	0.47
1:A:294:PRO:C	1:A:295:LEU:O	2.57	0.47
2:B:143:ARG:CB	2:B:143:ARG:NH1	2.76	0.47
1:A:25:PRO:CG	1:A:133:PRO:HG2	2.45	0.46
1:A:130:PHE:CE1	1:A:146:TYR:CE2	3.03	0.46
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.45	0.46
1:A:258:GLN:NE2	1:A:283:LEU:CD2	2.75	0.46
2:B:28:GLU:O	2:B:29:GLU:C	2.57	0.46
1:A:257:ILE:HG23	1:A:279:LEU:HD23	1.97	0.46
1:A:440:PHE:CE2	1:A:457:TYR:CZ	2.98	0.46
1:A:129:ALA:HA	1:A:145:GLN:HA	1.98	0.46
1:A:183:TYR:O	1:A:186:ASP:HB2	2.15	0.46
2:B:12:LEU:CD2	2:B:124:PHE:HE2	2.28	0.46
2:B:28:GLU:O	2:B:31:ILE:HG23	2.16	0.46
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.97	0.46
2:B:201:LYS:O	2:B:204:GLU:HB3	2.15	0.46
2:B:206:ARG:HG2	2:B:217:PRO:CG	2.29	0.46
1:A:235:HIS:O	1:A:238:LYS:O	2.34	0.46
2:B:142:ILE:N	2:B:142:ILE:HD12	2.30	0.46
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.98	0.46
1:A:114:ALA:C	1:A:116:PHE:N	2.74	0.46
1:A:264:LEU:HD12	1:A:276:VAL:HG22	1.98	0.46
1:A:461:LYS:C	1:A:463:ARG:H	2.23	0.46
1:A:222:GLN:O	1:A:223:LYS:CB	2.63	0.46
1:A:242:GLN:CB	1:A:243:PRO:CD	2.92	0.46
2:B:388:LYS:HA	2:B:413:GLU:O	2.16	0.46
1:A:13:LYS:HG3	1:A:84:THR:CA	2.46	0.46
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.31	0.46
1:A:460:ASN:HA	2:B:286:THR:HG21	1.98	0.46
1:A:506:ILE:H	1:A:506:ILE:CD1	2.29	0.46
2:B:11:LYS:HZ1	2:B:124:PHE:HD2	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:ALA:O	2:B:300:GLU:C	2.57	0.46
2:B:369:THR:HG22	2:B:370:GLU:N	2.31	0.46
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.50	0.46
1:A:210:LEU:HA	1:A:213:GLY:O	2.16	0.46
1:A:276:VAL:O	1:A:277:ARG:C	2.58	0.46
1:A:421:PRO:O	1:A:423:VAL:N	2.49	0.46
2:B:164:MET:SD	2:B:168:LEU:CD1	3.02	0.46
2:B:398:TRP:O	2:B:402:TRP:HD1	1.99	0.46
1:A:206:ARG:CZ	1:A:206:ARG:HB3	2.46	0.46
1:A:460:ASN:HA	2:B:286:THR:CG2	2.45	0.46
2:B:13:LYS:HB2	2:B:87:PHE:CG	2.51	0.46
2:B:153:TRP:CE3	2:B:155:GLY:HA3	2.50	0.46
2:B:293:ILE:HG22	2:B:295:LEU:HD12	1.97	0.46
1:A:180:ILE:HG21	1:A:189:VAL:HG22	1.97	0.45
1:A:326:ILE:N	1:A:343:GLN:HE22	2.14	0.45
1:A:329:ILE:CB	1:A:390:LYS:HB2	2.45	0.45
1:A:420:PRO:HA	1:A:421:PRO:HD2	1.46	0.45
2:B:66:LYS:N	2:B:407:GLN:NE2	2.64	0.45
2:B:91:GLN:O	2:B:92:LEU:CB	2.63	0.45
2:B:191:SER:OG	2:B:198:HIS:CD2	2.67	0.45
2:B:252:TRP:CB	2:B:294:PRO:HB3	2.45	0.45
2:B:286:THR:CG2	2:B:287:LYS:N	2.79	0.45
2:B:401:TRP:CD1	2:B:401:TRP:N	2.83	0.45
1:A:435:VAL:HG12	2:B:289:LEU:HB3	1.98	0.45
2:B:88:TRP:O	2:B:88:TRP:CD1	2.70	0.45
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.81	0.45
1:A:41:MET:O	1:A:47:ILE:N	2.49	0.45
1:A:101:LYS:HE3	1:A:322:SER:OG	2.17	0.45
1:A:183:TYR:O	1:A:184:MET:O	2.33	0.45
1:A:285:GLY:O	1:A:287:LYS:N	2.50	0.45
1:A:484:LEU:HA	1:A:484:LEU:HD13	1.63	0.45
1:A:538:ALA:O	1:A:539:HIS:HB3	2.16	0.45
2:B:11:LYS:NZ	2:B:12:LEU:CD2	2.77	0.45
2:B:286:THR:O	2:B:287:LYS:HB2	2.17	0.45
2:B:379:SER:O	2:B:383:TRP:N	2.50	0.45
1:A:213:GLY:O	1:A:214:LEU:C	2.58	0.45
1:A:374:LYS:O	1:A:378:GLU:HB2	2.15	0.45
1:A:412:PRO:HD3	2:B:401:TRP:HH2	1.82	0.45
1:A:442:VAL:CG2	1:A:495:ILE:HG23	2.46	0.45
1:A:80:LEU:O	1:A:81:ASN:C	2.60	0.45
1:A:438:GLU:OE2	1:A:461:LYS:HD3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:PHE:CZ	2:B:151:GLN:CB	3.00	0.45
2:B:337:TRP:HH2	2:B:364:ASP:HB2	1.81	0.45
1:A:164:MET:SD	1:A:214:LEU:HD13	2.56	0.45
1:A:265:ASN:O	1:A:266:TRP:C	2.60	0.45
1:A:122:GLU:C	1:A:124:PHE:H	2.25	0.45
1:A:386:THR:HG21	1:A:412:PRO:HG2	1.97	0.45
1:A:443:ASP:HB2	1:A:548:VAL:CG1	2.47	0.45
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.99	0.45
2:B:17:ASP:O	2:B:83:ARG:HD3	2.17	0.45
1:A:100:LEU:HD21	3:A:557:NVP:C5	2.47	0.45
1:A:200:THR:O	1:A:203:GLU:N	2.49	0.45
1:A:492:GLU:O	1:A:493:VAL:HG12	2.17	0.45
1:A:535:TRP:CG	1:A:536:VAL:N	2.85	0.45
2:B:24:TRP:CZ3	2:B:25:PRO:O	2.70	0.45
1:A:430:GLU:O	1:A:532:TYR:HD1	2.00	0.45
2:B:22:LYS:O	2:B:23:GLN:CB	2.65	0.45
2:B:150:PRO:HB2	2:B:153:TRP:CD1	2.52	0.45
2:B:368:LEU:O	2:B:372:VAL:HG12	2.16	0.45
1:A:30:LYS:O	1:A:31:ILE:C	2.59	0.44
1:A:33:ALA:HB1	1:A:71:TRP:HB3	1.99	0.44
1:A:447:ASN:HD22	1:A:450:THR:H	1.65	0.44
2:B:380:ILE:HD11	2:B:386:THR:HG22	1.99	0.44
1:A:341:ILE:O	1:A:349:LEU:HB2	2.16	0.44
2:B:23:GLN:HE22	2:B:26:LEU:HG	1.83	0.44
2:B:63:ILE:O	2:B:72:ARG:N	2.49	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.85	0.44
1:A:13:LYS:HG3	1:A:84:THR:HA	1.99	0.44
1:A:52:PRO:CA	1:A:143:ARG:HB2	2.48	0.44
1:A:80:LEU:HD22	1:A:153:TRP:NE1	2.32	0.44
1:A:260:LEU:O	1:A:264:LEU:HG	2.17	0.44
1:A:492:GLU:HB3	1:A:493:VAL:H	1.51	0.44
1:A:505:ILE:HG22	1:A:506:ILE:HD13	1.98	0.44
2:B:21:VAL:HG12	2:B:22:LYS:N	2.32	0.44
2:B:65:LYS:C	2:B:66:LYS:HD3	2.43	0.44
2:B:183:TYR:CD1	2:B:183:TYR:C	2.93	0.44
2:B:293:ILE:HB	2:B:295:LEU:H	1.82	0.44
1:A:125:ARG:CD	1:A:147:ASN:HA	2.44	0.44
1:A:318:TYR:O	1:A:319:TYR:HB2	2.17	0.44
1:A:432:GLU:HA	1:A:433:PRO:HD2	1.66	0.44
1:A:442:VAL:HG13	1:A:481:ALA:HB1	2.00	0.44
2:B:395:LYS:O	2:B:396:GLU:CB	2.62	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD12	1:A:84:THR:HG23	2.00	0.44
1:A:37:ILE:HG22	1:A:38:CYS:N	2.32	0.44
1:A:163:SER:O	1:A:167:ILE:HG13	2.17	0.44
1:A:473:THR:CB	1:A:476:LYS:HE3	2.48	0.44
1:A:501:TYR:CD1	1:A:501:TYR:C	2.94	0.44
2:B:217:PRO:O	2:B:219:LYS:O	2.36	0.44
2:B:254:VAL:HG13	2:B:255:ASN:N	2.32	0.44
1:A:160:PHE:O	1:A:162:SER:N	2.50	0.44
1:A:167:ILE:HD13	1:A:214:LEU:CD1	2.48	0.44
1:A:200:THR:C	1:A:202:ILE:H	2.25	0.44
1:A:497:THR:O	1:A:536:VAL:HG12	2.18	0.44
1:A:80:LEU:HD21	1:A:124:PHE:HZ	1.83	0.44
1:A:289:LEU:O	1:A:291:GLU:N	2.51	0.44
1:A:321:PRO:O	1:A:322:SER:O	2.35	0.44
1:A:442:VAL:HG13	1:A:481:ALA:O	2.17	0.44
2:B:195:ILE:C	2:B:197:GLN:N	2.74	0.44
2:B:218:ASP:O	2:B:219:LYS:HB3	2.18	0.44
1:A:427:TYR:OH	1:A:509:GLN:C	2.61	0.44
1:A:450:THR:HB	1:A:452:LEU:HG	1.99	0.44
2:B:40:GLU:HG3	2:B:43:LYS:NZ	2.33	0.44
2:B:85:GLN:O	2:B:89:GLU:N	2.51	0.44
2:B:286:THR:CG2	2:B:287:LYS:H	2.28	0.44
1:A:38:CYS:HA	1:A:41:MET:CG	2.48	0.44
1:A:60:VAL:HG21	1:A:131:THR:O	2.18	0.44
1:A:387:PRO:HG2	1:A:389:PHE:CE2	2.51	0.44
2:B:423:VAL:C	2:B:425:LEU:N	2.75	0.44
1:A:11:LYS:N	1:A:87:PHE:CE2	2.78	0.43
1:A:99:GLY:O	1:A:320:ASP:HB2	2.17	0.43
1:A:395:LYS:O	1:A:398:TRP:N	2.51	0.43
1:A:398:TRP:CH2	1:A:411:ILE:CG2	3.01	0.43
2:B:51:GLY:HA2	2:B:52:PRO:HD3	1.66	0.43
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.40	0.43
2:B:220:LYS:H	2:B:220:LYS:HG2	1.54	0.43
1:A:47:ILE:HG23	1:A:148:VAL:HG21	1.99	0.43
1:A:334:GLN:C	1:A:336:GLN:H	2.24	0.43
1:A:395:LYS:O	1:A:396:GLU:C	2.61	0.43
1:A:548:VAL:HG13	1:A:549:ASP:N	2.32	0.43
2:B:46:LYS:O	2:B:147:ASN:HB2	2.18	0.43
2:B:301:LEU:HD13	2:B:301:LEU:O	2.18	0.43
1:A:128:THR:O	1:A:145:GLN:HA	2.19	0.43
1:A:208:HIS:O	1:A:212:TRP:CD1	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:C	2:B:71:TRP:HE3	2.26	0.43
2:B:147:ASN:N	2:B:147:ASN:ND2	2.56	0.43
2:B:78:ARG:NH1	2:B:413:GLU:HA	2.33	0.43
1:A:12:LEU:HA	1:A:84:THR:HG22	1.97	0.43
1:A:111:VAL:HG22	1:A:216:THR:HG23	2.00	0.43
1:A:203:GLU:HA	1:A:206:ARG:HH12	1.83	0.43
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.86	0.43
1:A:411:ILE:HA	1:A:412:PRO:HD3	1.85	0.43
2:B:116:PHE:CZ	2:B:151:GLN:HB3	2.53	0.43
1:A:77:PHE:CZ	1:A:150:PRO:CB	3.01	0.43
1:A:183:TYR:C	1:A:184:MET:O	2.59	0.43
1:A:422:LEU:O	1:A:424:LYS:N	2.51	0.43
1:A:446:ALA:HA	1:A:452:LEU:O	2.19	0.43
2:B:278:GLN:NE2	2:B:281:LYS:NZ	2.67	0.43
1:A:97:PRO:C	1:A:99:GLY:N	2.76	0.43
1:A:138:GLU:O	1:A:140:PRO:HD3	2.19	0.43
1:A:275:LYS:HE3	1:A:275:LYS:HB3	1.64	0.43
1:A:329:ILE:HA	1:A:390:LYS:O	2.18	0.43
1:A:340:GLN:HB2	1:A:348:ASN:ND2	2.33	0.43
1:A:443:ASP:OD2	1:A:549:ASP:HA	2.19	0.43
1:A:521:ILE:O	1:A:525:LEU:HG	2.19	0.43
2:B:149:LEU:HD21	2:B:159:ILE:CG2	2.48	0.43
2:B:263:LYS:O	2:B:267:ALA:N	2.49	0.43
2:B:366:LYS:HZ3	2:B:369:THR:HG21	1.84	0.43
1:A:5:ILE:CG2	1:A:6:GLU:H	2.31	0.43
1:A:220:LYS:O	1:A:221:HIS:CB	2.66	0.43
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.43
1:A:503:LEU:HD12	1:A:504:GLY:H	1.80	0.43
2:B:107:THR:HG1	2:B:198:HIS:CE1	2.36	0.43
1:A:40:GLU:C	1:A:42:GLU:N	2.76	0.43
1:A:138:GLU:O	1:A:140:PRO:CD	2.67	0.43
1:A:233:GLU:OE2	1:A:242:GLN:HG3	2.18	0.43
1:A:271:TYR:CD1	1:A:314:VAL:CB	3.01	0.43
1:A:328:GLU:O	1:A:389:PHE:HA	2.19	0.43
2:B:119:PRO:HG2	2:B:149:LEU:HD13	2.01	0.43
2:B:173:LYS:C	2:B:175:ASN:N	2.73	0.43
2:B:23:GLN:HE21	2:B:133:PRO:HG2	1.83	0.43
2:B:210:LEU:O	2:B:213:GLY:O	2.36	0.43
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.62	0.42
1:A:200:THR:HA	1:A:203:GLU:HG3	2.01	0.42
2:B:402:TRP:H	2:B:402:TRP:CD1	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD22	1:A:264:LEU:HG	2.00	0.42
1:A:353:LYS:HE3	1:A:353:LYS:HB2	1.85	0.42
1:A:450:THR:C	1:A:452:LEU:H	2.27	0.42
1:A:491:LEU:HD13	1:A:529:GLU:OE2	2.19	0.42
1:A:539:HIS:HA	1:A:545:ASN:OD1	2.19	0.42
2:B:207:GLN:O	2:B:211:ARG:HG3	2.20	0.42
1:A:235:HIS:C	1:A:237:ASP:N	2.77	0.42
1:A:421:PRO:C	1:A:423:VAL:N	2.77	0.42
1:A:525:LEU:O	1:A:527:LYS:N	2.52	0.42
2:B:206:ARG:CG	2:B:217:PRO:HG2	2.30	0.42
1:A:117:SER:OG	1:A:118:VAL:N	2.51	0.42
1:A:434:ILE:HG21	1:A:492:GLU:HG3	2.02	0.42
1:A:484:LEU:O	1:A:485:ALA:C	2.62	0.42
2:B:125:ARG:H	2:B:125:ARG:HD2	1.84	0.42
2:B:160:PHE:O	2:B:160:PHE:CD2	2.72	0.42
1:A:171:PHE:O	1:A:174:GLN:N	2.52	0.42
1:A:286:THR:O	1:A:288:ALA:N	2.52	0.42
1:A:362:THR:HG22	1:A:366:LYS:CB	2.48	0.42
2:B:13:LYS:HA	2:B:87:PHE:CD2	2.55	0.42
2:B:13:LYS:HA	2:B:87:PHE:CE2	2.54	0.42
2:B:101:LYS:O	2:B:104:LYS:HG2	2.20	0.42
2:B:122:GLU:O	2:B:123:ASP:CB	2.67	0.42
2:B:143:ARG:HB3	2:B:143:ARG:NH1	2.24	0.42
2:B:427:TYR:CD2	2:B:428:GLN:HG3	2.55	0.42
1:A:103:LYS:HA	1:A:192:ASP:OD1	2.18	0.42
1:A:258:GLN:HE21	1:A:283:LEU:HD11	1.84	0.42
1:A:521:ILE:O	1:A:521:ILE:HG22	2.20	0.42
2:B:46:LYS:HB3	2:B:148:VAL:CG1	2.48	0.42
2:B:208:HIS:HD2	2:B:211:ARG:NH2	2.17	0.42
1:A:183:TYR:CE2	1:A:230:MET:HE2	2.51	0.42
1:A:239:TRP:CZ3	1:A:317:VAL:CB	3.00	0.42
1:A:270:ILE:HD12	1:A:315:HIS:HA	2.02	0.42
1:A:320:ASP:HA	1:A:321:PRO:HD3	1.84	0.42
1:A:520:GLN:C	1:A:522:ILE:N	2.77	0.42
2:B:50:ILE:HA	2:B:144:TYR:HA	2.02	0.42
2:B:192:ASP:O	2:B:194:GLU:HG2	2.20	0.42
2:B:268:SER:HA	2:B:271:TYR:HD2	1.84	0.42
2:B:286:THR:O	2:B:287:LYS:CB	2.67	0.42
1:A:132:ILE:HB	1:A:142:ILE:CB	2.49	0.42
1:A:389:PHE:HB2	1:A:414:TRP:HA	2.01	0.42
1:A:461:LYS:C	1:A:463:ARG:N	2.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:SER:HB3	2:B:4:PRO:HA	2.02	0.42
2:B:92:LEU:HD23	2:B:92:LEU:HA	1.97	0.42
2:B:379:SER:OG	2:B:387:PRO:HD3	2.19	0.42
1:A:16:MET:H	1:A:16:MET:HG2	1.57	0.42
1:A:185:ASP:O	1:A:186:ASP:CG	2.63	0.42
1:A:298:GLU:O	1:A:299:ALA:C	2.62	0.42
1:A:322:SER:O	1:A:323:LYS:CB	2.68	0.42
1:A:374:LYS:O	1:A:378:GLU:CB	2.68	0.42
1:A:506:ILE:O	1:A:509:GLN:N	2.49	0.42
2:B:65:LYS:HG3	2:B:72:ARG:HD2	2.01	0.42
2:B:116:PHE:CZ	2:B:151:GLN:HB2	2.55	0.42
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.34	0.42
2:B:205:LEU:O	2:B:205:LEU:HD12	2.19	0.42
2:B:397:THR:O	2:B:401:TRP:CD1	2.73	0.42
1:A:80:LEU:CD2	1:A:153:TRP:HE1	2.33	0.42
1:A:234:LEU:HD11	3:A:557:NVP:HCD2	2.01	0.42
1:A:460:ASN:HB3	2:B:286:THR:HG22	2.02	0.42
1:A:527:LYS:HG3	1:A:527:LYS:O	2.20	0.42
2:B:5:ILE:O	2:B:6:GLU:CG	2.63	0.42
2:B:172:LYS:O	2:B:176:PRO:HA	2.20	0.42
2:B:194:GLU:O	2:B:196:GLY:N	2.52	0.42
1:A:97:PRO:O	1:A:98:ALA:C	2.60	0.41
1:A:171:PHE:HA	1:A:174:GLN:NE2	2.35	0.41
1:A:241:VAL:CG1	1:A:266:TRP:CD1	3.03	0.41
1:A:255:ASN:O	1:A:259:LYS:HG3	2.20	0.41
2:B:369:THR:CG2	2:B:370:GLU:N	2.83	0.41
1:A:132:ILE:O	1:A:133:PRO:C	2.62	0.41
1:A:296:THR:CG2	1:A:299:ALA:H	2.32	0.41
2:B:13:LYS:HE3	2:B:14:PRO:O	2.20	0.41
1:A:214:LEU:HD23	1:A:214:LEU:H	1.85	0.41
1:A:276:VAL:HG12	1:A:276:VAL:O	2.19	0.41
1:A:458:VAL:CG2	1:A:551:LEU:HD11	2.50	0.41
2:B:411:ILE:HA	2:B:412:PRO:HD2	1.92	0.41
1:A:334:GLN:C	1:A:336:GLN:N	2.75	0.41
1:A:385:LYS:HE3	1:A:385:LYS:HB3	1.80	0.41
1:A:96:HIS:HD2	1:A:97:PRO:CD	2.25	0.41
1:A:106:VAL:HG12	1:A:190:GLY:HA3	2.02	0.41
1:A:317:VAL:C	1:A:319:TYR:H	2.27	0.41
1:A:350:LYS:HD3	1:A:351:THR:N	2.34	0.41
1:A:463:ARG:O	1:A:464:GLN:NE2	2.54	0.41
2:B:206:ARG:HH21	2:B:218:ASP:HA	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:ARG:C	2:B:213:GLY:H	2.28	0.41
2:B:282:LEU:CG	2:B:292:VAL:HG11	2.48	0.41
1:A:12:LEU:HD12	1:A:84:THR:CG2	2.51	0.41
1:A:38:CYS:HA	1:A:41:MET:HG2	2.03	0.41
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.86	0.41
2:B:10:VAL:HG13	2:B:88:TRP:CE2	2.56	0.41
2:B:277:ARG:C	2:B:280:CYS:HB3	2.46	0.41
2:B:284:ARG:HD2	2:B:284:ARG:N	2.35	0.41
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.41
1:A:398:TRP:CE3	1:A:402:TRP:HD1	2.38	0.41
2:B:49:LYS:O	2:B:145:GLN:N	2.53	0.41
2:B:263:LYS:HA	2:B:263:LYS:HD3	1.72	0.41
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.01	0.41
1:A:398:TRP:CZ3	1:A:411:ILE:HG21	2.55	0.41
1:A:465:LYS:CG	1:A:466:VAL:N	2.84	0.41
1:A:492:GLU:O	1:A:493:VAL:CB	2.69	0.41
1:A:520:GLN:C	1:A:522:ILE:H	2.27	0.41
2:B:58:THR:HA	2:B:59:PRO:HD3	1.93	0.41
2:B:257:ILE:HG23	2:B:261:VAL:CG2	2.50	0.41
2:B:301:LEU:O	2:B:302:GLU:HB2	2.20	0.41
2:B:304:ALA:O	2:B:305:GLU:C	2.63	0.41
2:B:390:LYS:HB3	2:B:417:VAL:CG1	2.51	0.41
1:A:5:ILE:CG2	1:A:6:GLU:N	2.83	0.41
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.86	0.41
1:A:160:PHE:O	1:A:161:GLN:C	2.62	0.41
1:A:171:PHE:O	1:A:175:ASN:OD1	2.39	0.41
1:A:239:TRP:CG	1:A:240:THR:N	2.88	0.41
1:A:343:GLN:HB2	1:A:349:LEU:HD12	2.02	0.41
1:A:393:ILE:HG23	1:A:394:GLN:N	2.35	0.41
1:A:395:LYS:O	1:A:397:THR:N	2.54	0.41
1:A:451:LYS:O	1:A:470:THR:HA	2.21	0.41
2:B:42:GLU:OE1	2:B:144:TYR:HE1	2.04	0.41
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.56	0.41
2:B:418:ASN:OD1	2:B:418:ASN:N	2.54	0.41
2:B:425:LEU:HG	2:B:428:GLN:OXT	2.21	0.41
1:A:445:ALA:N	1:A:477:THR:OG1	2.54	0.41
1:A:548:VAL:CG1	1:A:549:ASP:N	2.84	0.41
2:B:293:ILE:CG2	2:B:295:LEU:N	2.84	0.41
2:B:395:LYS:HG3	2:B:416:PHE:CD2	2.56	0.41
1:A:64:LYS:CB	1:A:72:ARG:HD3	2.51	0.40
1:A:206:ARG:NH1	1:A:206:ARG:HB3	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:O	2:B:44:GLU:N	2.52	0.40
2:B:65:LYS:O	2:B:66:LYS:HB2	2.21	0.40
1:A:26:LEU:HB2	1:A:30:LYS:HB2	2.02	0.40
1:A:63:ILE:O	1:A:71:TRP:CD1	2.74	0.40
1:A:269:GLN:O	1:A:351:THR:HB	2.20	0.40
1:A:381:VAL:HG22	2:B:25:PRO:CB	2.52	0.40
2:B:13:LYS:HG2	2:B:14:PRO:CD	2.51	0.40
2:B:332:GLN:HA	2:B:337:TRP:CE2	2.56	0.40
2:B:365:VAL:C	2:B:367:GLN:H	2.29	0.40
1:A:247:PRO:O	1:A:247:PRO:HG2	2.21	0.40
1:A:406:TRP:CD1	1:A:406:TRP:O	2.74	0.40
1:A:453:GLY:N	1:A:469:LEU:O	2.49	0.40
2:B:417:VAL:O	2:B:417:VAL:CG1	2.69	0.40
1:A:300:GLU:O	1:A:304:ALA:CB	2.68	0.40
1:A:365:VAL:HG22	1:A:393:ILE:HD11	2.03	0.40
2:B:156:SER:O	2:B:159:ILE:N	2.54	0.40
2:B:368:LEU:CD2	2:B:393:ILE:HD12	2.49	0.40
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.45	0.40
1:A:94:ILE:HD11	1:A:230:MET:HG2	2.03	0.40
1:A:112:GLY:N	1:A:217:PRO:HD3	2.36	0.40
1:A:224:GLU:CD	1:A:226:PRO:HD2	2.46	0.40
1:A:339:TYR:CD1	1:A:339:TYR:C	3.00	0.40
1:A:550:LYS:O	1:A:551:LEU:C	2.64	0.40
2:B:166:LYS:HD2	2:B:166:LYS:HA	1.83	0.40
2:B:217:PRO:O	2:B:218:ASP:C	2.65	0.40
2:B:304:ALA:CA	2:B:307:ARG:HB3	2.45	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:CG1	1:A:449:GLU:OE2[4_647]	1.87	0.33
1:A:37:ILE:CD1	1:A:449:GLU:OE2[4_647]	1.99	0.21
1:A:4:PRO:CB	2:B:211:ARG:NH2[4_646]	2.08	0.12
1:A:70:LYS:NZ	1:A:449:GLU:OE2[4_647]	2.09	0.11

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	553/556 (100%)	338 (61%)	125 (23%)	90 (16%)	0	0
2	B	392/428 (92%)	264 (67%)	62 (16%)	66 (17%)	0	0
All	All	945/984 (96%)	602 (64%)	187 (20%)	156 (16%)	0	0

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	25	PRO
1	A	54	ASN
1	A	66	LYS
1	A	121	ASP
1	A	125	ARG
1	A	145	GLN
1	A	185	ASP
1	A	221	HIS
1	A	226	PRO
1	A	242	GLN
1	A	248	GLU
1	A	251	SER
1	A	276	VAL
1	A	286	THR
1	A	288	ALA
1	A	290	THR
1	A	311	LYS
1	A	321	PRO
1	A	322	SER
1	A	325	LEU
1	A	345	PRO
1	A	346	PHE
1	A	354	TYR
1	A	363	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	395	LYS
1	A	396	GLU
1	A	419	THR
1	A	421	PRO
1	A	424	LYS
1	A	457	TYR
1	A	471	ASN
1	A	492	GLU
1	A	538	ALA
2	B	4	PRO
2	B	6	GLU
2	B	21	VAL
2	B	46	LYS
2	B	52	PRO
2	B	68	SER
2	B	104	LYS
2	B	117	SER
2	B	141	GLY
2	B	193	LEU
2	B	195	ILE
2	B	198	HIS
2	B	281	LYS
2	B	287	LYS
2	B	293	ILE
2	B	295	LEU
2	B	302	GLU
2	B	312	GLU
2	B	315	HIS
2	B	321	PRO
2	B	323	LYS
2	B	334	GLN
2	B	345	PRO
2	B	346	PHE
2	B	420	PRO
2	B	425	LEU
2	B	426	TRP
1	A	30	LYS
1	A	71	TRP
1	A	75	VAL
1	A	115	TYR
1	A	172	LYS
1	A	184	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	ILE
1	A	210	LEU
1	A	214	LEU
1	A	223	LYS
1	A	247	PRO
1	A	283	LEU
1	A	285	GLY
1	A	295	LEU
1	A	310	LEU
1	A	316	GLY
1	A	323	LYS
1	A	462	GLY
1	A	493	VAL
1	A	512	LYS
1	A	516	GLU
1	A	540	LYS
2	B	23	GLN
2	B	47	ILE
2	B	66	LYS
2	B	92	LEU
2	B	116	PHE
2	B	177	ASP
2	B	212	TRP
2	B	218	ASP
2	B	280	CYS
2	B	317	VAL
2	B	322	SER
2	B	396	GLU
1	A	43	LYS
1	A	57	ASN
1	A	63	ILE
1	A	77	PHE
1	A	122	GLU
1	A	134	SER
1	A	215	THR
1	A	246	LEU
1	A	281	LYS
1	A	304	ALA
1	A	423	VAL
1	A	510	PRO
1	A	529	GLU
1	A	539	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	553	SER
2	B	45	GLY
2	B	91	GLN
2	B	105	SER
2	B	119	PRO
2	B	133	PRO
2	B	200	THR
2	B	251	SER
2	B	350	LYS
2	B	403	THR
1	A	27	THR
1	A	55	PRO
1	A	87	PHE
1	A	186	ASP
1	A	287	LYS
1	A	312	GLU
1	A	433	PRO
1	A	464	GLN
2	B	184	MET
2	B	211	ARG
1	A	64	LYS
1	A	113	ASP
1	A	227	PHE
1	A	250	ASP
1	A	530	LYS
2	B	355	ALA
2	B	408	ALA
2	B	427	TYR
1	A	31	ILE
1	A	225	PRO
1	A	292	VAL
2	B	219	LYS
2	B	268	SER
2	B	276	VAL
2	B	423	VAL
1	A	333	GLY
1	A	526	ILE
2	B	25	PRO
2	B	271	TYR
2	B	9	PRO
2	B	261	VAL
2	B	273	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	152	GLY
2	B	421	PRO
2	B	262	GLY
1	A	314	VAL
2	B	294	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/496 (16%)	64 (79%)	17 (21%)	1	4
2	B	328/390 (84%)	235 (72%)	93 (28%)	0	1
All	All	409/886 (46%)	299 (73%)	110 (27%)	0	1

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	349	LEU
1	A	357	MET
1	A	363	ASN
1	A	373	GLN
1	A	416	PHE
1	A	419	THR
1	A	464	GLN
1	A	466	VAL
1	A	523	GLU
1	A	524	GLN
1	A	533	LEU
1	A	536	VAL
1	A	537	PRO
1	A	546	GLU
2	B	2	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	5	ILE
2	B	11	LYS
2	B	12	LEU
2	B	16	MET
2	B	21	VAL
2	B	22	LYS
2	B	23	GLN
2	B	25	PRO
2	B	26	LEU
2	B	28	GLU
2	B	31	ILE
2	B	44	GLU
2	B	46	LYS
2	B	47	ILE
2	B	54	ASN
2	B	55	PRO
2	B	65	LYS
2	B	66	LYS
2	B	69	THR
2	B	78	ARG
2	B	82	LYS
2	B	91	GLN
2	B	108	VAL
2	B	119	PRO
2	B	120	LEU
2	B	121	ASP
2	B	125	ARG
2	B	128	THR
2	B	143	ARG
2	B	147	ASN
2	B	154	LYS
2	B	159	ILE
2	B	162	SER
2	B	165	THR
2	B	168	LEU
2	B	175	ASN
2	B	177	ASP
2	B	178	ILE
2	B	189	VAL
2	B	192	ASP
2	B	193	LEU
2	B	195	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	206	ARG
2	B	212	TRP
2	B	215	THR
2	B	216	THR
2	B	218	ASP
2	B	219	LYS
2	B	220	LYS
2	B	222	GLN
2	B	223	LYS
2	B	252	TRP
2	B	253	THR
2	B	254	VAL
2	B	255	ASN
2	B	258	GLN
2	B	265	ASN
2	B	274	ILE
2	B	275	LYS
2	B	277	ARG
2	B	278	GLN
2	B	279	LEU
2	B	280	CYS
2	B	282	LEU
2	B	284	ARG
2	B	289	LEU
2	B	291	GLU
2	B	293	ILE
2	B	295	LEU
2	B	301	LEU
2	B	303	LEU
2	B	312	GLU
2	B	337	TRP
2	B	354	TYR
2	B	366	LYS
2	B	367	GLN
2	B	369	THR
2	B	376	THR
2	B	377	THR
2	B	380	ILE
2	B	381	VAL
2	B	393	ILE
2	B	401	TRP
2	B	403	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	414	TRP
2	B	418	ASN
2	B	420	PRO
2	B	423	VAL
2	B	424	LYS
2	B	425	LEU
2	B	427	TYR
2	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	343	GLN
1	A	363	ASN
1	A	520	GLN
1	A	524	GLN
2	B	23	GLN
2	B	54	ASN
2	B	57	ASN
2	B	147	ASN
2	B	198	HIS
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	373	GLN
2	B	407	GLN
2	B	428	GLN

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NVP	A	557	-	23,23,23	1.77	3 (13%)	34,34,34	1.71	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NVP	A	557	-	-	0/4/6/6	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	NVP	C9-N8	6.97	1.41	1.35
3	A	557	NVP	OE-C9	-3.39	1.15	1.23
3	A	557	NVP	C7-N8	2.03	1.44	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	NVP	C10-C9-N8	-6.62	113.76	120.22
3	A	557	NVP	OE-C9-C10	4.57	124.19	119.61
3	A	557	NVP	C7-N8-C9	2.82	130.61	128.29
3	A	557	NVP	C15-N1-CA	-2.30	114.52	116.34
3	A	557	NVP	C15-C10-C9	2.10	126.06	124.01

There are no chirality outliers.

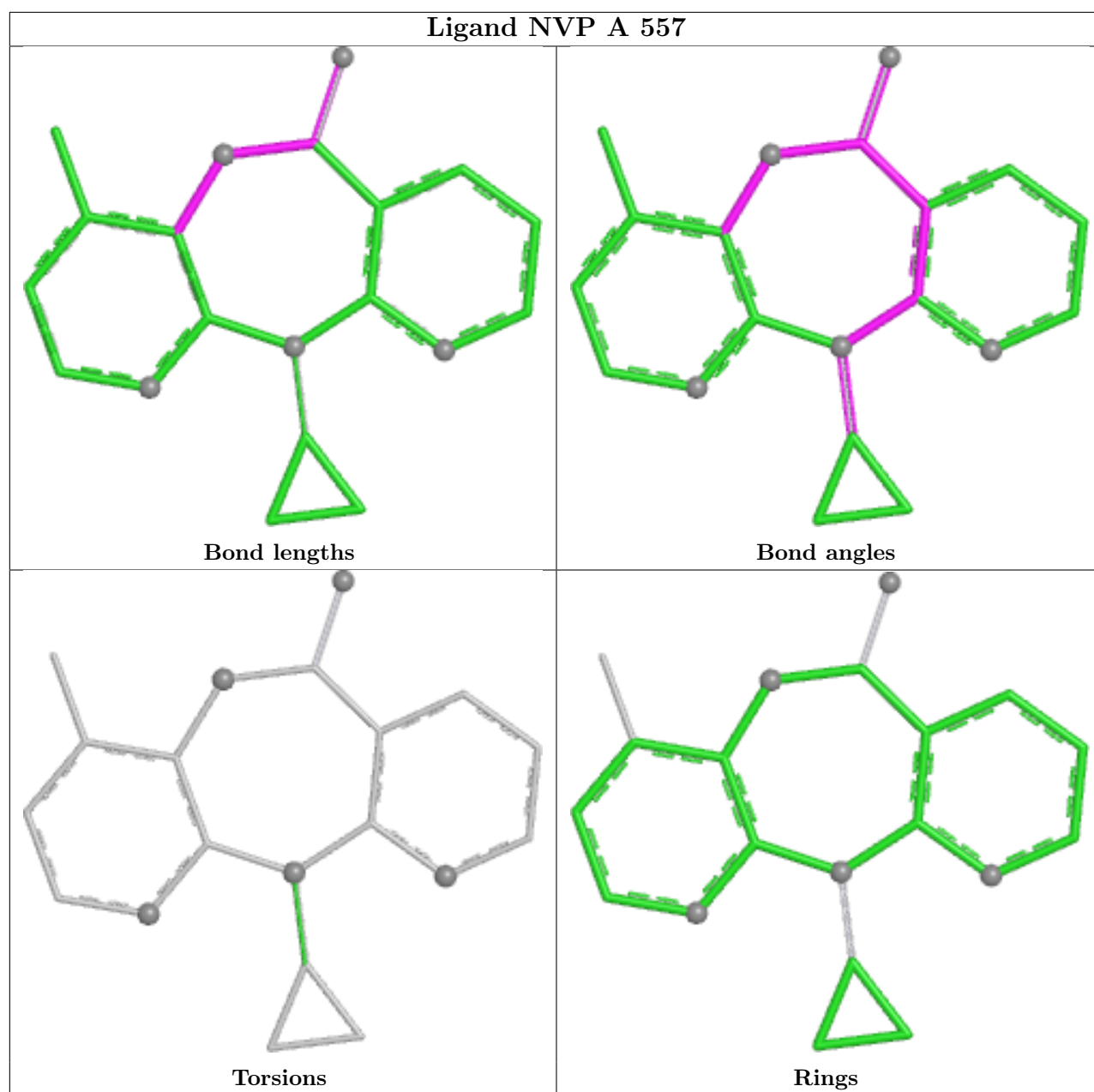
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	NVP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.