



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:44 AM UTC

PDB ID : 1BQN / pdb_00001bqn
Title : TYR 188 LEU HIV-1 RT/HBY 097
Authors : Hsiou, Y.; Das, K.; Ding, J.; Arnold, E.
Deposited on : 1998-08-17
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
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

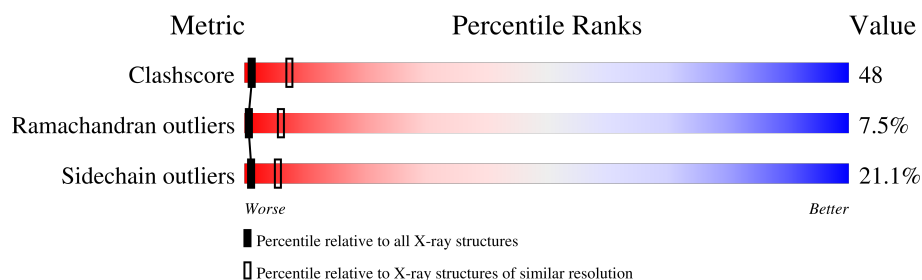
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	558	
2	B	430	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7834 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4372	2825	729	811	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	TYR	engineered mutation	UNP P03366
A	248	GLN	GLU	conflict	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	546	GLN	GLU	conflict	UNP P03366

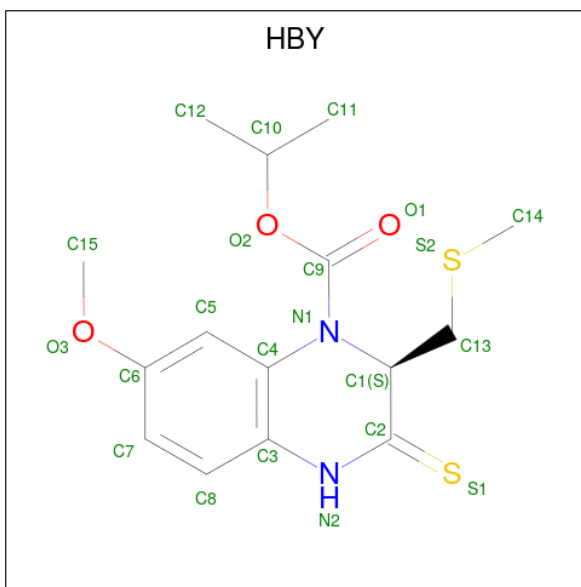
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3440	2239	568	628	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	LEU	TYR	engineered mutation	UNP P03366
B	242	GLU	GLN	conflict	UNP P03366
B	278	ALA	GLN	conflict	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is (S)-4-ISOPROPOXYCARBONYL-6-METHOXY-3-METHYLTHIOMETHYL-3,4-DIHYDROQUINOXALIN-2(1H)-THIONE (CCD ID: HBY) (formula: C₁₅H₂₀N₂O₃S₂).



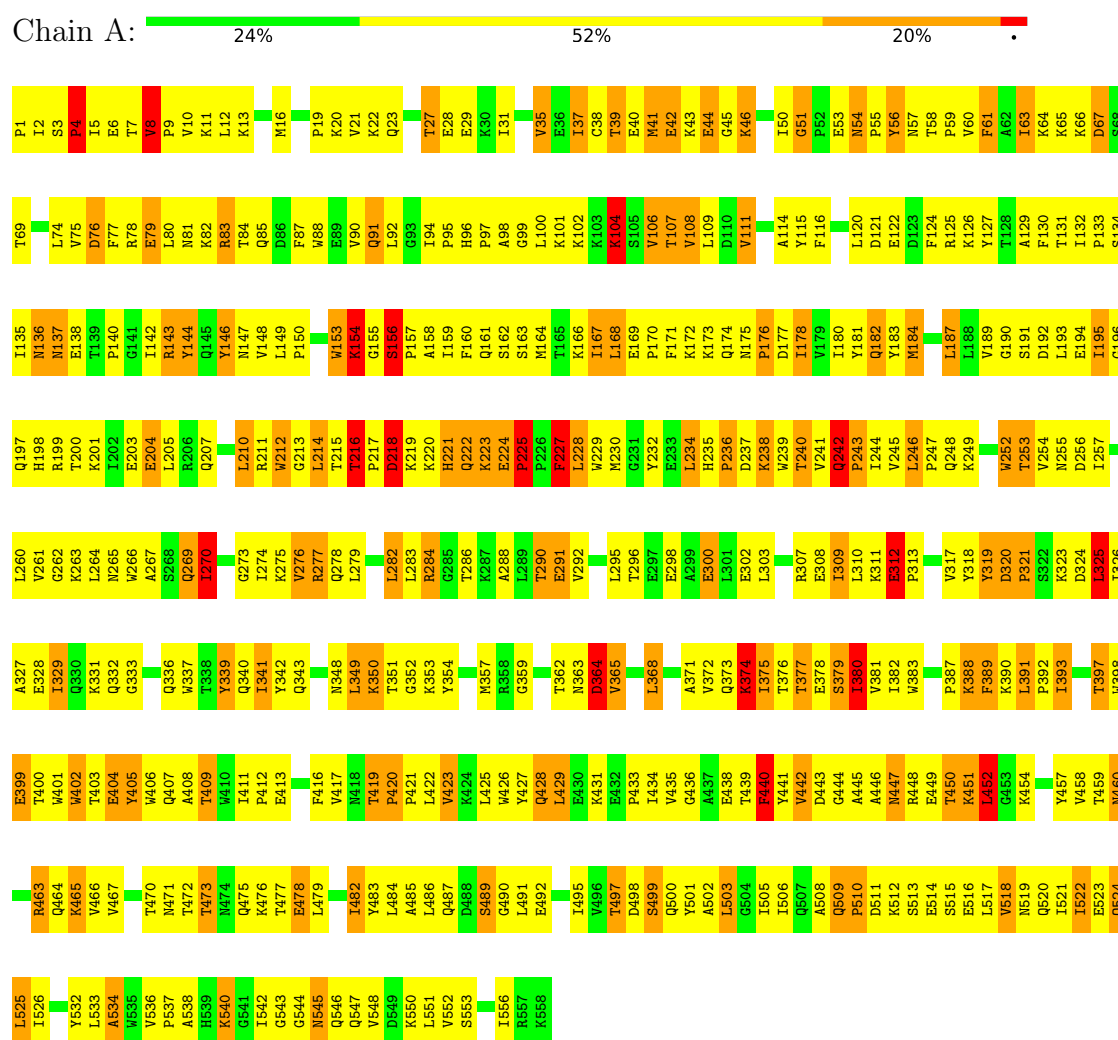
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	22	15	2	3	2	0	0

3 Residue-property plots

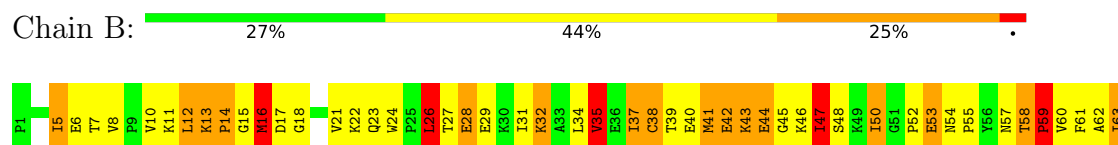
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: REVERSE TRANSCRIPTASE





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	224.80Å 69.30Å 105.30Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	95.1 (10.00-3.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.245 , 0.362	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7834	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: HBY

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	0.97	3/4487 (0.1%)	1.54	89/6118 (1.5%)
2	B	1.04	4/3539 (0.1%)	1.61	95/4825 (2.0%)
All	All	1.00	7/8026 (0.1%)	1.57	184/10943 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	MET	SD-CE	8.94	2.02	1.79
1	A	225	PRO	CA-C	6.72	1.58	1.52
1	A	375	ILE	CA-CB	6.31	1.61	1.54
2	B	139	THR	CA-CB	5.88	1.63	1.53
2	B	5	ILE	CA-CB	5.85	1.62	1.54
1	A	447	ASN	CA-CB	-5.27	1.46	1.52
2	B	150	PRO	CA-C	-5.16	1.46	1.52

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	PRO	N-CA-C	17.68	132.26	110.70
1	A	224	GLU	CA-C-N	15.05	135.88	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	C-N-CA	15.05	135.88	120.38
1	A	8	VAL	CA-C-N	13.00	136.09	119.84
1	A	8	VAL	C-N-CA	13.00	136.09	119.84
2	B	316	GLY	N-CA-C	-11.92	84.93	113.18
2	B	215	THR	N-CA-C	-11.55	91.95	110.32
1	A	216	THR	CA-C-N	11.51	134.23	119.84
1	A	216	THR	C-N-CA	11.51	134.23	119.84
2	B	89	GLU	N-CA-C	-10.99	99.90	113.97
2	B	344	GLU	CA-C-N	10.25	132.65	119.84
2	B	344	GLU	C-N-CA	10.25	132.65	119.84
2	B	391	LEU	N-CA-C	10.10	122.35	109.72
1	A	227	PHE	N-CA-C	10.09	125.45	108.20
1	A	54	ASN	CA-C-N	9.83	129.47	119.24
1	A	54	ASN	C-N-CA	9.83	129.47	119.24
1	A	312	GLU	CA-C-N	9.79	132.08	119.84
1	A	312	GLU	C-N-CA	9.79	132.08	119.84
2	B	185	ASP	N-CA-C	-9.76	99.03	112.30
1	A	388	LYS	N-CA-C	-9.56	96.33	110.48
1	A	320	ASP	CA-C-N	9.36	131.54	119.84
1	A	320	ASP	C-N-CA	9.36	131.54	119.84
2	B	386	THR	CA-C-N	9.31	129.25	119.85
2	B	386	THR	C-N-CA	9.31	129.25	119.85
1	A	380	ILE	N-CA-C	-9.29	103.82	111.81
2	B	7	THR	N-CA-C	9.28	125.10	110.17
2	B	87	PHE	N-CA-C	-9.28	104.05	114.62
2	B	366	LYS	N-CA-C	-9.11	101.30	111.14
1	A	83	ARG	N-CA-C	8.90	120.67	110.97
2	B	158	ALA	N-CA-C	-8.86	101.31	110.97
2	B	388	LYS	N-CA-C	-8.51	96.23	109.25
1	A	536	VAL	N-CA-C	8.48	116.14	109.19
2	B	357	MET	N-CA-C	8.38	121.15	110.33
2	B	426	TRP	N-CA-C	-8.38	96.33	109.07
2	B	175	ASN	CA-C-N	8.28	130.19	119.84
2	B	175	ASN	C-N-CA	8.28	130.19	119.84
2	B	84	THR	N-CA-C	8.15	119.86	110.97
2	B	94	ILE	CA-C-N	8.13	127.89	119.76
2	B	94	ILE	C-N-CA	8.13	127.89	119.76
1	A	42	GLU	N-CA-C	-8.10	102.45	111.28
2	B	233	GLU	N-CA-C	8.04	122.13	107.99
1	A	276	VAL	N-CA-C	-8.02	105.67	113.53
1	A	536	VAL	CA-C-N	8.02	129.86	119.84
1	A	536	VAL	C-N-CA	8.02	129.86	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	LYS	N-CA-C	-7.92	102.33	110.97
1	A	497	THR	N-CA-C	7.90	122.11	109.24
2	B	414	TRP	N-CA-C	7.84	120.99	109.07
2	B	143	ARG	N-CA-C	7.83	121.49	108.73
1	A	167	ILE	N-CA-C	7.80	117.91	110.42
2	B	149	LEU	CA-C-N	7.68	128.13	119.83
2	B	149	LEU	C-N-CA	7.68	128.13	119.83
2	B	279	LEU	N-CA-C	-7.61	102.56	112.68
2	B	42	GLU	N-CA-C	-7.57	102.99	112.90
2	B	393	ILE	N-CA-C	7.49	116.84	107.70
2	B	401	TRP	N-CA-C	7.47	124.15	113.02
2	B	376	THR	N-CA-C	7.45	123.67	111.37
1	A	499	SER	N-CA-C	7.42	122.42	109.96
2	B	86	ASP	N-CA-C	-7.37	103.60	112.59
2	B	94	ILE	N-CA-C	-7.37	92.97	108.88
2	B	263	LYS	N-CA-C	-7.33	103.23	111.07
2	B	64	LYS	N-CA-C	-7.27	93.42	107.44
1	A	288	ALA	N-CA-C	7.24	119.67	110.33
1	A	556	ILE	N-CA-C	7.20	119.37	109.80
2	B	35	VAL	N-CA-C	-7.17	103.98	111.58
1	A	553	SER	N-CA-C	7.16	120.78	110.10
1	A	290	THR	N-CA-C	-7.15	106.47	114.62
1	A	391	LEU	CA-C-N	7.14	128.77	119.84
1	A	391	LEU	C-N-CA	7.14	128.77	119.84
1	A	440	PHE	N-CA-C	7.11	120.51	107.99
2	B	132	ILE	CA-C-N	7.11	127.03	119.85
2	B	132	ILE	C-N-CA	7.11	127.03	119.85
1	A	325	LEU	N-CA-C	-7.08	97.36	108.90
1	A	214	LEU	N-CA-C	7.06	120.44	109.07
2	B	58	THR	CA-C-N	6.99	127.02	119.89
2	B	58	THR	C-N-CA	6.99	127.02	119.89
1	A	503	LEU	N-CA-C	-6.95	103.64	111.07
1	A	35	VAL	N-CA-C	-6.93	103.02	110.23
2	B	174	GLN	N-CA-C	-6.91	103.85	112.90
2	B	99	GLY	N-CA-C	-6.89	103.62	115.61
1	A	178	ILE	N-CA-C	-6.80	102.53	110.21
1	A	364	ASP	N-CA-C	6.76	118.54	111.03
2	B	250	ASP	N-CA-C	6.76	120.08	110.68
1	A	69	THR	N-CA-C	6.76	118.65	111.28
1	A	115	TYR	N-CA-C	-6.73	105.07	113.55
1	A	204	GLU	N-CA-C	-6.66	103.94	111.07
1	A	420	PRO	N-CA-C	6.61	118.77	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	VAL	N-CA-C	6.53	116.97	108.35
1	A	223	LYS	N-CA-C	6.48	119.87	110.28
2	B	48	SER	N-CA-C	6.47	119.03	108.55
2	B	417	VAL	N-CA-C	6.46	117.66	108.93
1	A	514	GLU	N-CA-C	-6.40	105.44	113.18
2	B	352	GLY	N-CA-C	6.39	119.84	110.38
2	B	344	GLU	N-CA-C	-6.39	95.69	109.81
1	A	11	LYS	N-CA-C	-6.37	99.72	109.41
2	B	246	LEU	N-CA-C	-6.35	102.06	109.93
1	A	348	ASN	N-CA-C	6.33	118.48	108.67
2	B	12	LEU	N-CA-C	6.30	118.86	109.59
1	A	63	ILE	N-CA-C	6.28	122.39	109.34
2	B	28	GLU	N-CA-C	-6.27	103.75	111.40
2	B	8	VAL	CA-C-N	6.24	127.64	119.84
2	B	8	VAL	C-N-CA	6.24	127.64	119.84
2	B	259	LYS	N-CA-C	-6.11	104.24	111.03
2	B	372	VAL	N-CA-C	6.10	116.76	110.36
2	B	204	GLU	N-CA-C	-6.07	103.82	111.11
1	A	27	THR	O-C-N	6.05	129.57	121.83
2	B	35	VAL	CB-CA-C	-6.03	104.34	111.94
2	B	189	VAL	CA-C-N	-6.02	116.40	121.58
2	B	189	VAL	C-N-CA	-6.02	116.40	121.58
1	A	284	ARG	N-CA-C	5.99	123.55	110.80
2	B	13	LYS	CA-C-N	5.95	127.28	119.84
2	B	13	LYS	C-N-CA	5.95	127.28	119.84
1	A	402	TRP	N-CA-C	-5.94	99.03	110.56
2	B	324	ASP	N-CA-C	5.94	118.10	108.41
1	A	61	PHE	N-CA-C	-5.93	99.73	109.40
1	A	41	MET	N-CA-C	-5.93	104.21	112.45
2	B	276	VAL	N-CA-C	5.89	121.59	109.34
2	B	375	ILE	CB-CA-C	-5.89	101.63	111.29
2	B	18	GLY	CA-C-N	5.84	126.18	119.93
2	B	18	GLY	C-N-CA	5.84	126.18	119.93
1	A	309	ILE	N-CA-C	-5.84	104.64	110.30
1	A	218	ASP	N-CA-C	5.83	123.23	110.80
2	B	254	VAL	CB-CA-C	-5.80	104.22	112.22
2	B	251	SER	N-CA-C	-5.78	103.81	112.54
2	B	189	VAL	N-CA-C	5.78	116.19	107.75
1	A	391	LEU	N-CA-C	5.78	119.60	108.45
2	B	47	ILE	N-CA-C	5.75	117.46	109.29
2	B	224	GLU	N-CA-C	-5.72	102.69	110.36
1	A	500	GLN	N-CA-C	-5.72	102.18	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	THR	CA-C-N	-5.69	118.38	123.33
2	B	131	THR	C-N-CA	-5.69	118.38	123.33
2	B	198	HIS	N-CA-C	-5.65	105.26	111.82
1	A	172	LYS	N-CA-C	-5.65	105.65	112.54
2	B	270	ILE	CB-CA-C	5.65	120.55	111.29
1	A	419	THR	CA-C-N	5.64	126.19	120.38
1	A	419	THR	C-N-CA	5.64	126.19	120.38
2	B	303	LEU	N-CA-C	-5.62	104.55	111.40
1	A	452	LEU	N-CA-C	5.59	118.81	110.14
2	B	371	ALA	N-CA-C	-5.58	105.11	111.14
1	A	309	ILE	CB-CA-C	-5.57	104.84	111.81
1	A	525	LEU	N-CA-C	-5.57	104.42	111.11
1	A	161	GLN	N-CA-C	-5.54	105.32	111.36
2	B	429	LEU	N-CA-C	5.52	117.77	107.99
1	A	136	ASN	CB-CA-C	-5.51	104.44	111.22
1	A	451	LYS	N-CA-C	5.50	122.53	110.80
1	A	374	LYS	CA-C-N	5.50	127.43	120.72
1	A	374	LYS	C-N-CA	5.50	127.43	120.72
1	A	434	ILE	N-CA-C	5.49	116.13	108.89
2	B	254	VAL	N-CA-C	-5.48	105.18	110.72
2	B	38	CYS	N-CA-C	5.48	119.47	112.34
1	A	365	VAL	N-CA-C	-5.45	104.64	110.36
2	B	169	GLU	N-CA-C	5.44	121.84	109.81
1	A	156	SER	CA-C-N	5.38	125.20	119.28
1	A	156	SER	C-N-CA	5.38	125.20	119.28
2	B	59	PRO	N-CA-C	5.36	119.63	111.11
1	A	51	GLY	CA-C-N	5.34	125.41	119.32
1	A	51	GLY	C-N-CA	5.34	125.41	119.32
1	A	269	GLN	N-CA-C	-5.30	105.17	111.69
1	A	245	VAL	N-CA-C	5.27	120.30	109.34
1	A	409	THR	N-CA-C	5.27	117.19	109.24
2	B	154	LYS	N-CA-C	-5.26	107.03	113.50
2	B	16	MET	N-CA-C	5.23	117.08	110.33
1	A	534	ALA	N-CA-C	-5.23	100.79	108.79
1	A	389	PHE	N-CA-C	5.20	117.38	108.90
1	A	64	LYS	CB-CA-C	-5.19	100.09	110.42
1	A	212	TRP	N-CA-C	5.17	119.22	113.02
2	B	77	PHE	N-CA-C	-5.12	107.05	113.15
1	A	270	ILE	N-CA-C	5.12	119.99	109.34
2	B	295	LEU	N-CA-C	5.12	117.29	110.53
2	B	26	LEU	N-CA-C	5.12	115.80	108.74
1	A	524	GLN	N-CA-C	-5.10	105.61	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	N-CA-C	5.05	117.73	109.59
2	B	239	TRP	N-CA-C	5.05	121.57	110.80
2	B	309	ILE	N-CA-C	-5.05	105.48	112.50
2	B	382	ILE	N-CA-C	5.05	116.47	111.67
2	B	242	GLU	CA-C-N	5.04	126.15	119.84
2	B	242	GLU	C-N-CA	5.04	126.15	119.84
1	A	82	LYS	N-CA-C	-5.04	105.43	111.03
1	A	329	ILE	N-CA-C	5.04	115.17	108.11
1	A	253	THR	N-CA-C	-5.02	102.36	110.14
2	B	289	LEU	N-CA-C	5.02	117.64	111.82
2	B	315	HIS	N-CA-CB	5.02	118.97	110.49
1	A	13	LYS	CA-C-N	5.01	126.11	119.84
1	A	13	LYS	C-N-CA	5.01	126.11	119.84
2	B	114	ALA	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	TYR	Sidechain
2	B	183	TYR	Sidechain
2	B	316	GLY	Mainchain
2	B	346	PHE	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	4372	0	4271	428	0
2	B	3440	0	3400	327	0
3	A	22	0	20	8	0
All	All	7834	0	7691	743	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (743) 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)
2:B:41:MET:SD	2:B:41:MET:CE	2.01	1.48
1:A:97:PRO:HG2	1:A:232:TYR:CE2	1.66	1.29
1:A:27:THR:O	1:A:31:ILE:HG13	1.41	1.15
2:B:38:CYS:HB3	2:B:144:TYR:CE2	1.84	1.11
2:B:38:CYS:HB3	2:B:144:TYR:HE2	0.93	1.05
1:A:242:GLN:HB3	1:A:243:PRO:HD3	1.39	1.00
1:A:183:TYR:CE2	1:A:184:MET:HG2	1.97	1.00
1:A:229:TRP:HB3	1:A:234:LEU:HD11	1.43	0.99
1:A:191:SER:OG	1:A:198:HIS:HD2	1.47	0.98
2:B:400:THR:HG22	2:B:401:TRP:CD1	1.99	0.98
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.42	0.98
2:B:400:THR:HG22	2:B:401:TRP:HD1	1.24	0.97
1:A:108:VAL:HA	1:A:187:LEU:O	1.65	0.96
1:A:97:PRO:CG	1:A:232:TYR:CE2	2.49	0.95
1:A:40:GLU:HA	1:A:43:LYS:HB2	1.49	0.94
1:A:240:THR:HG22	1:A:241:VAL:H	1.26	0.94
2:B:125:ARG:HG2	2:B:146:TYR:O	1.71	0.91
1:A:229:TRP:HB3	1:A:234:LEU:CD1	2.00	0.90
2:B:368:LEU:O	2:B:372:VAL:HG23	1.73	0.88
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.57	0.87
2:B:242:GLU:N	2:B:243:PRO:HD3	1.90	0.86
2:B:198:HIS:O	2:B:202:ILE:HG12	1.76	0.85
1:A:10:VAL:HG12	1:A:124:PHE:HE2	1.43	0.84
1:A:278:GLN:O	1:A:282:LEU:HD23	1.76	0.84
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.58	0.84
2:B:358:ARG:HH11	2:B:358:ARG:HB3	1.41	0.83
1:A:224:GLU:CB	1:A:225:PRO:HD2	2.09	0.83
1:A:107:THR:HG21	1:A:221:HIS:O	1.79	0.82
1:A:10:VAL:HG12	1:A:124:PHE:CE2	2.14	0.82
2:B:319:TYR:HD1	2:B:343:GLN:HE22	1.25	0.81
1:A:21:VAL:HG12	1:A:22:LYS:H	1.44	0.81
1:A:377:THR:O	1:A:381:VAL:HG23	1.81	0.81
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.11	0.80
2:B:23:GLN:NE2	2:B:26:LEU:HD21	1.97	0.80
1:A:183:TYR:CD2	1:A:184:MET:HG2	2.16	0.79
1:A:66:LYS:O	1:A:67:ASP:CB	2.30	0.79
1:A:3:SER:HA	1:A:213:GLY:HA3	1.64	0.79
2:B:303:LEU:O	2:B:307:ARG:HB2	1.84	0.78
1:A:438:GLU:HB3	1:A:440:PHE:HE1	1.48	0.78
2:B:423:VAL:O	2:B:425:LEU:HG	1.84	0.78
1:A:253:THR:HA	1:A:292:VAL:HA	1.65	0.78
1:A:3:SER:OG	1:A:5:ILE:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD12	1:A:75:VAL:H	1.49	0.78
1:A:459:THR:CG2	1:A:463:ARG:HB3	2.13	0.78
1:A:9:PRO:HG2	2:B:53:GLU:HG2	1.64	0.78
1:A:331:LYS:HG2	1:A:333:GLY:H	1.46	0.77
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.64	0.77
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.19	0.77
1:A:97:PRO:CG	1:A:232:TYR:CD2	2.68	0.77
2:B:275:LYS:HB3	2:B:302:GLU:OE2	1.85	0.77
1:A:131:THR:HG22	1:A:143:ARG:HB3	1.67	0.76
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.65	0.76
1:A:164:MET:HE1	1:A:168:LEU:HD21	1.66	0.76
2:B:109:LEU:HD12	2:B:187:LEU:HD23	1.69	0.75
1:A:19:PRO:O	1:A:56:TYR:HB3	1.85	0.75
2:B:341:ILE:HD12	2:B:350:LYS:HB3	1.66	0.75
2:B:167:ILE:O	2:B:208:HIS:HE1	1.70	0.75
1:A:240:THR:HG22	1:A:241:VAL:N	2.00	0.74
2:B:210:LEU:HD11	2:B:216:THR:HG23	1.69	0.74
3:A:559:HBY:C9	3:A:559:HBY:S2	2.75	0.74
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.51	0.74
1:A:27:THR:O	1:A:31:ILE:CG1	2.31	0.74
2:B:275:LYS:O	2:B:302:GLU:HB3	1.88	0.74
2:B:271:TYR:O	2:B:274:ILE:HG13	1.88	0.73
2:B:78:ARG:HD3	2:B:411:ILE:O	1.88	0.73
1:A:260:LEU:HD21	1:A:279:LEU:HD22	1.69	0.72
1:A:326:ILE:HG23	1:A:342:TYR:CE1	2.24	0.72
1:A:483:TYR:HE1	1:A:524:GLN:NE2	1.86	0.72
1:A:195:ILE:O	1:A:199:ARG:HG3	1.89	0.72
1:A:253:THR:OG1	1:A:255:ASN:HB3	1.90	0.72
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.24	0.72
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.70	0.72
1:A:132:ILE:O	1:A:142:ILE:HB	1.90	0.71
1:A:482:ILE:HG22	1:A:495:ILE:HD13	1.70	0.71
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.71	0.71
1:A:401:TRP:CZ3	1:A:404:GLU:HG2	2.25	0.71
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.73	0.70
1:A:240:THR:CG2	1:A:241:VAL:H	2.04	0.70
1:A:365:VAL:O	1:A:368:LEU:HB3	1.92	0.70
2:B:375:ILE:HG13	2:B:389:PHE:CE1	2.26	0.70
1:A:382:ILE:HG23	2:B:136:ASN:OD1	1.91	0.69
1:A:454:LYS:HB2	1:A:552:VAL:HG13	1.73	0.69
1:A:518:VAL:HA	1:A:521:ILE:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLY:HA3	3:A:559:HBX:H143	1.73	0.69
1:A:328:GLU:HA	1:A:390:LYS:O	1.92	0.69
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.20	0.69
1:A:97:PRO:HG3	1:A:232:TYR:CD2	2.28	0.68
2:B:27:THR:O	2:B:31:ILE:HG13	1.94	0.68
1:A:339:TYR:CE1	1:A:352:GLY:N	2.61	0.68
1:A:246:LEU:CD1	1:A:264:LEU:HD21	2.24	0.68
2:B:79:GLU:O	2:B:83:ARG:HG2	1.92	0.68
2:B:63:ILE:HG22	2:B:64:LYS:H	1.59	0.68
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.58	0.68
1:A:257:ILE:O	1:A:261:VAL:HG23	1.95	0.67
2:B:375:ILE:HG13	2:B:389:PHE:HE1	1.57	0.67
1:A:457:TYR:HE1	1:A:465:LYS:HD3	1.59	0.67
2:B:107:THR:OG1	2:B:198:HIS:HE1	1.77	0.67
2:B:239:TRP:N	2:B:239:TRP:HE3	1.92	0.67
2:B:243:PRO:O	2:B:245:VAL:HG23	1.95	0.67
2:B:258:GLN:NE2	2:B:289:LEU:HD21	2.10	0.67
2:B:38:CYS:CB	2:B:144:TYR:HE2	1.88	0.66
2:B:158:ALA:O	2:B:161:GLN:HB2	1.95	0.66
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.77	0.66
1:A:502:ALA:O	1:A:506:ILE:HD12	1.95	0.66
2:B:132:ILE:HG13	2:B:142:ILE:O	1.95	0.66
1:A:182:GLN:HE21	1:A:183:TYR:N	1.92	0.66
1:A:326:ILE:HG23	1:A:342:TYR:CD1	2.30	0.66
2:B:37:ILE:HG22	2:B:38:CYS:N	2.10	0.66
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.31	0.66
1:A:445:ALA:O	1:A:477:THR:HG21	1.95	0.66
2:B:369:THR:HA	2:B:398:TRP:HH2	1.61	0.66
1:A:544:GLY:HA3	2:B:286:THR:HG23	1.77	0.66
1:A:300:GLU:HA	1:A:303:LEU:HB3	1.79	0.65
1:A:428:GLN:C	1:A:429:LEU:HD23	2.21	0.65
1:A:483:TYR:O	1:A:486:LEU:HB2	1.95	0.65
1:A:241:VAL:HG23	1:A:270:ILE:HD11	1.77	0.65
2:B:63:ILE:HG22	2:B:64:LYS:N	2.11	0.65
1:A:31:ILE:O	1:A:35:VAL:HG23	1.97	0.65
1:A:4:PRO:HD2	1:A:212:TRP:O	1.97	0.65
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.79	0.65
2:B:41:MET:SD	2:B:47:ILE:HD13	2.37	0.65
1:A:57:ASN:OD1	1:A:130:PHE:HA	1.97	0.64
2:B:50:ILE:HD11	2:B:144:TYR:C	2.22	0.64
2:B:356:ARG:HA	2:B:356:ARG:NE	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:CB	2:B:14:PRO:HD2	2.26	0.64
2:B:128:THR:HB	2:B:146:TYR:HB2	1.78	0.64
2:B:97:PRO:O	2:B:100:LEU:HB2	1.97	0.64
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.25	0.64
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.79	0.64
2:B:183:TYR:O	2:B:186:ASP:HB2	1.96	0.64
1:A:191:SER:OG	1:A:198:HIS:CD2	2.39	0.64
1:A:53:GLU:O	1:A:55:PRO:HD3	1.97	0.63
1:A:324:ASP:O	1:A:343:GLN:HG2	1.98	0.63
2:B:65:LYS:HG3	2:B:66:LYS:N	2.13	0.63
2:B:239:TRP:N	2:B:239:TRP:CE3	2.67	0.63
2:B:21:VAL:HG12	2:B:22:LYS:N	2.14	0.63
1:A:248:GLN:HG3	1:A:249:LYS:H	1.63	0.63
1:A:248:GLN:HG3	1:A:249:LYS:N	2.14	0.63
2:B:410:TRP:HE3	2:B:410:TRP:O	1.82	0.63
2:B:65:LYS:HG3	2:B:66:LYS:H	1.63	0.63
1:A:341:ILE:O	1:A:349:LEU:HB3	1.99	0.62
2:B:116:PHE:HD1	2:B:148:VAL:HG21	1.63	0.62
1:A:515:SER:OG	1:A:518:VAL:HG23	2.00	0.62
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.63	0.62
1:A:100:LEU:HD11	3:A:559:HB:Y:H111	1.81	0.62
2:B:238:LYS:C	2:B:239:TRP:HE3	2.08	0.62
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.33	0.62
1:A:246:LEU:HD12	1:A:264:LEU:HD21	1.80	0.62
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.67	0.62
1:A:216:THR:HG22	1:A:218:ASP:OD2	2.00	0.62
1:A:164:MET:CE	1:A:168:LEU:HD21	2.30	0.61
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.81	0.61
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.30	0.61
1:A:435:VAL:HG12	2:B:290:THR:HG21	1.81	0.61
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.31	0.61
1:A:96:HIS:CE1	1:A:98:ALA:H	2.18	0.61
2:B:425:LEU:HD12	2:B:426:TRP:H	1.64	0.61
1:A:109:LEU:HB2	1:A:187:LEU:HB3	1.83	0.61
1:A:326:ILE:HG13	1:A:388:LYS:O	1.99	0.61
2:B:164:MET:HE3	2:B:168:LEU:HG	1.83	0.61
2:B:164:MET:HG3	2:B:168:LEU:HD11	1.81	0.61
1:A:228:LEU:H	1:A:228:LEU:CD2	2.14	0.61
1:A:327:ALA:HB2	1:A:341:ILE:HG23	1.82	0.61
1:A:50:ILE:HG13	1:A:51:GLY:H	1.66	0.61
1:A:40:GLU:CA	1:A:43:LYS:HB2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HG3	1:A:148:VAL:HG21	1.83	0.60
1:A:479:LEU:O	1:A:482:ILE:HG13	2.01	0.60
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.16	0.60
1:A:12:LEU:HD23	1:A:84:THR:HA	1.83	0.60
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.01	0.60
1:A:5:ILE:HD12	1:A:6:GLU:HG3	1.84	0.60
2:B:78:ARG:NH1	2:B:411:ILE:HG22	2.16	0.60
1:A:1:PRO:HD2	1:A:44:GLU:HB3	1.82	0.60
1:A:194:GLU:O	1:A:196:GLY:N	2.35	0.60
1:A:181:TYR:OH	1:A:183:TYR:HB2	2.02	0.60
1:A:372:VAL:O	1:A:375:ILE:HB	2.01	0.60
2:B:37:ILE:CG2	2:B:38:CYS:N	2.65	0.60
1:A:429:LEU:HD13	1:A:533:LEU:HD13	1.83	0.60
2:B:107:THR:HG22	2:B:108:VAL:N	2.17	0.60
2:B:78:ARG:NH1	2:B:412:PRO:O	2.35	0.60
2:B:329:ILE:HG22	2:B:330:GLN:N	2.16	0.60
1:A:375:ILE:HG21	1:A:389:PHE:CZ	2.37	0.59
1:A:146:TYR:CD1	1:A:150:PRO:HG3	2.37	0.59
1:A:513:SER:HB2	1:A:519:ASN:OD1	2.02	0.59
2:B:160:PHE:O	2:B:160:PHE:CD1	2.56	0.59
1:A:244:ILE:HD11	1:A:267:ALA:HB2	1.84	0.59
1:A:265:ASN:HD21	1:A:353:LYS:NZ	2.01	0.59
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.20	0.59
1:A:460:ASN:H	1:A:460:ASN:HD22	1.49	0.59
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.68	0.59
2:B:126:LYS:HG3	2:B:127:TYR:CE1	2.37	0.59
2:B:242:GLU:H	2:B:243:PRO:HD3	1.68	0.59
2:B:344:GLU:O	2:B:347:LYS:HB2	2.03	0.58
1:A:114:ALA:O	1:A:160:PHE:HE2	1.86	0.58
1:A:153:TRP:HZ3	1:A:159:ILE:HD12	1.68	0.58
1:A:166:LYS:O	1:A:169:GLU:HB3	2.03	0.58
2:B:303:LEU:HD21	2:B:307:ARG:NH1	2.18	0.58
1:A:484:LEU:HA	1:A:487:GLN:OE1	2.04	0.58
2:B:391:LEU:HD12	2:B:414:TRP:HB2	1.85	0.58
2:B:375:ILE:HG21	2:B:389:PHE:CZ	2.38	0.58
2:B:329:ILE:HG23	2:B:338:THR:O	2.04	0.58
1:A:131:THR:C	1:A:133:PRO:HD3	2.28	0.58
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.34	0.58
1:A:254:VAL:CG1	1:A:283:LEU:HD11	2.34	0.58
2:B:132:ILE:HG22	2:B:133:PRO:HD2	1.85	0.58
2:B:257:ILE:HD13	2:B:282:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:TYR:CD2	2:B:383:TRP:CD1	2.92	0.58
1:A:96:HIS:CD2	1:A:232:TYR:OH	2.57	0.57
1:A:483:TYR:HE1	1:A:524:GLN:HE21	1.49	0.57
2:B:244:ILE:HG22	2:B:244:ILE:O	2.04	0.57
2:B:260:LEU:O	2:B:264:LEU:HG	2.03	0.57
2:B:268:SER:O	2:B:272:PRO:HA	2.05	0.57
1:A:56:TYR:CD1	1:A:56:TYR:N	2.69	0.57
1:A:106:VAL:HG13	1:A:189:VAL:O	2.05	0.57
1:A:46:LYS:HG2	1:A:116:PHE:HD2	1.68	0.57
1:A:253:THR:O	1:A:257:ILE:HG13	2.04	0.57
2:B:115:TYR:N	2:B:115:TYR:CD1	2.72	0.57
1:A:171:PHE:CD1	1:A:175:ASN:OD1	2.58	0.56
2:B:410:TRP:O	2:B:410:TRP:CE3	2.58	0.56
1:A:235:HIS:ND1	1:A:238:LYS:HG3	2.20	0.56
1:A:266:TRP:CH2	1:A:269:GLN:NE2	2.73	0.56
1:A:131:THR:HG22	1:A:143:ARG:CD	2.35	0.56
2:B:61:PHE:HD2	2:B:74:LEU:HD23	1.69	0.56
1:A:483:TYR:HE1	1:A:524:GLN:CG	2.18	0.56
2:B:10:VAL:HA	2:B:88:TRP:CZ2	2.39	0.56
2:B:254:VAL:HB	2:B:289:LEU:HD23	1.87	0.56
1:A:116:PHE:O	1:A:148:VAL:HG21	2.06	0.56
1:A:254:VAL:HA	1:A:257:ILE:HD12	1.86	0.56
2:B:79:GLU:HG3	2:B:83:ARG:NH1	2.20	0.56
1:A:100:LEU:HD11	3:A:559:HBV:C11	2.35	0.56
2:B:329:ILE:HA	2:B:338:THR:O	2.06	0.56
2:B:424:LYS:O	2:B:425:LEU:C	2.49	0.56
1:A:363:ASN:OD1	1:A:364:ASP:N	2.39	0.56
2:B:264:LEU:HD13	2:B:276:VAL:CG1	2.36	0.56
1:A:114:ALA:O	1:A:160:PHE:CE2	2.59	0.56
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.35	0.55
1:A:21:VAL:HG12	1:A:22:LYS:N	2.17	0.55
1:A:375:ILE:CG2	1:A:389:PHE:HZ	2.20	0.55
1:A:501:TYR:O	1:A:505:ILE:HG13	2.06	0.55
2:B:247:PRO:HB2	2:B:250:ASP:CB	2.36	0.55
2:B:17:ASP:O	2:B:83:ARG:NE	2.39	0.55
2:B:125:ARG:HE	2:B:147:ASN:HA	1.71	0.55
2:B:131:THR:HG22	2:B:132:ILE:N	2.21	0.55
1:A:341:ILE:HD12	1:A:350:LYS:HB3	1.88	0.55
2:B:398:TRP:C	2:B:400:THR:H	2.14	0.55
1:A:108:VAL:CA	1:A:187:LEU:O	2.46	0.55
2:B:225:PRO:N	2:B:226:PRO:HD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:THR:O	2:B:381:VAL:HG23	2.06	0.55
1:A:319:TYR:CD1	1:A:320:ASP:N	2.74	0.55
1:A:319:TYR:HE1	1:A:343:GLN:NE2	2.04	0.55
1:A:372:VAL:HA	1:A:375:ILE:HD12	1.89	0.55
1:A:144:TYR:N	1:A:144:TYR:CD1	2.75	0.55
1:A:427:TYR:OH	1:A:509:GLN:HA	2.07	0.55
3:A:559:HBYS2	3:A:559:HBYSO1	2.65	0.55
2:B:191:SER:OG	2:B:198:HIS:HD2	1.89	0.55
1:A:337:TRP:N	1:A:337:TRP:CD1	2.76	0.54
1:A:339:TYR:CD1	1:A:339:TYR:C	2.86	0.54
1:A:398:TRP:O	1:A:400:THR:N	2.39	0.54
1:A:508:ALA:O	1:A:509:GLN:HG2	2.07	0.54
2:B:12:LEU:HD13	2:B:16:MET:O	2.07	0.54
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.42	0.54
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.07	0.54
1:A:420:PRO:HG2	1:A:421:PRO:HD2	1.89	0.54
2:B:136:ASN:O	2:B:136:ASN:ND2	2.41	0.54
1:A:509:GLN:N	1:A:510:PRO:HD3	2.22	0.54
2:B:26:LEU:HG	2:B:133:PRO:HG3	1.90	0.54
1:A:373:GLN:O	1:A:374:LYS:C	2.50	0.54
2:B:23:GLN:HE22	2:B:26:LEU:HD21	1.72	0.54
1:A:464:GLN:O	1:A:465:LYS:HB2	2.07	0.54
1:A:228:LEU:H	1:A:228:LEU:HD23	1.72	0.54
2:B:81:ASN:N	2:B:81:ASN:OD1	2.38	0.54
2:B:109:LEU:HB2	2:B:111:VAL:HG23	1.89	0.54
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.90	0.54
1:A:373:GLN:O	1:A:375:ILE:N	2.41	0.54
2:B:59:PRO:HB2	2:B:76:ASP:CB	2.37	0.54
2:B:367:GLN:O	2:B:371:ALA:N	2.40	0.54
2:B:394:GLN:HB3	2:B:397:THR:HB	1.88	0.54
1:A:1:PRO:CD	1:A:44:GLU:HG2	2.37	0.54
1:A:521:ILE:HG22	1:A:525:LEU:HD12	1.89	0.54
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.43	0.53
1:A:170:PRO:O	1:A:173:LYS:HB3	2.08	0.53
1:A:200:THR:OG1	1:A:201:LYS:N	2.41	0.53
1:A:319:TYR:CD2	1:A:383:TRP:HD1	2.26	0.53
1:A:375:ILE:HD13	1:A:389:PHE:HE1	1.74	0.53
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.43	0.53
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.44	0.53
2:B:40:GLU:O	2:B:43:LYS:HB2	2.08	0.53
1:A:109:LEU:N	1:A:187:LEU:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:HE2	1:A:332:GLN:HE21	1.73	0.53
1:A:521:ILE:HG22	1:A:525:LEU:CD1	2.39	0.53
1:A:43:LYS:C	1:A:45:GLY:H	2.16	0.53
1:A:339:TYR:C	1:A:339:TYR:HD1	2.16	0.53
1:A:482:ILE:CG2	1:A:495:ILE:HD13	2.39	0.53
2:B:124:PHE:O	2:B:126:LYS:N	2.42	0.53
1:A:1:PRO:HD2	1:A:44:GLU:HG2	1.90	0.53
1:A:96:HIS:N	2:B:136:ASN:HD21	2.06	0.53
2:B:193:LEU:HD13	2:B:197:GLN:HB3	1.89	0.53
2:B:356:ARG:HA	2:B:356:ARG:HE	1.73	0.53
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.44	0.53
2:B:85:GLN:O	2:B:89:GLU:HB2	2.09	0.53
1:A:429:LEU:HD23	1:A:429:LEU:N	2.24	0.53
2:B:154:LYS:HE2	2:B:184:MET:HE1	1.91	0.53
1:A:153:TRP:HE3	1:A:156:SER:H	1.56	0.52
1:A:178:ILE:HD11	1:A:189:VAL:HG12	1.89	0.52
1:A:342:TYR:HD1	1:A:342:TYR:O	1.92	0.52
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.39	0.52
2:B:126:LYS:HG3	2:B:127:TYR:CD1	2.44	0.52
1:A:398:TRP:C	1:A:400:THR:N	2.65	0.52
2:B:234:LEU:O	2:B:236:PRO:HD3	2.09	0.52
2:B:282:LEU:HD13	2:B:296:THR:HG22	1.92	0.52
1:A:111:VAL:O	1:A:114:ALA:HB3	2.08	0.52
2:B:78:ARG:CZ	2:B:411:ILE:HG22	2.39	0.52
1:A:101:LYS:NZ	1:A:321:PRO:HG3	2.25	0.52
1:A:181:TYR:CD1	1:A:181:TYR:C	2.88	0.52
1:A:193:LEU:O	1:A:198:HIS:HB2	2.09	0.52
1:A:279:LEU:HD12	1:A:302:GLU:OE1	2.10	0.52
1:A:100:LEU:CD1	3:A:559:HBX:H111	2.40	0.52
1:A:109:LEU:HD23	1:A:218:ASP:OD2	2.09	0.52
1:A:131:THR:O	1:A:133:PRO:HD3	2.10	0.52
1:A:252:TRP:H	1:A:252:TRP:CD1	2.28	0.52
1:A:393:ILE:HD13	1:A:398:TRP:HE3	1.75	0.52
1:A:96:HIS:HD2	1:A:232:TYR:OH	1.93	0.52
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.39	0.52
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.92	0.52
2:B:278:ALA:O	2:B:299:ALA:HB2	2.10	0.52
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.92	0.52
1:A:420:PRO:HG2	1:A:421:PRO:CD	2.39	0.52
2:B:179:VAL:HG12	2:B:180:ILE:N	2.25	0.52
1:A:393:ILE:CD1	1:A:398:TRP:HE3	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:O	1:A:200:THR:HG23	2.11	0.51
1:A:339:TYR:HD1	1:A:339:TYR:O	1.91	0.51
1:A:466:VAL:HG12	1:A:467:VAL:N	2.24	0.51
2:B:107:THR:HG22	2:B:108:VAL:H	1.75	0.51
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.10	0.51
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.93	0.51
2:B:277:ARG:O	2:B:279:LEU:N	2.43	0.51
1:A:12:LEU:HA	1:A:84:THR:HA	1.92	0.51
2:B:184:MET:HE3	2:B:410:TRP:HB3	1.92	0.51
1:A:244:ILE:O	1:A:244:ILE:HG23	2.11	0.51
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.92	0.51
1:A:542:ILE:HG12	1:A:545:ASN:CG	2.35	0.51
1:A:5:ILE:HD12	1:A:6:GLU:H	1.76	0.51
1:A:155:GLY:O	1:A:156:SER:C	2.54	0.51
1:A:252:TRP:CD1	1:A:252:TRP:N	2.78	0.51
2:B:191:SER:OG	2:B:198:HIS:CD2	2.63	0.51
1:A:406:TRP:CG	1:A:407:GLN:H	2.28	0.51
1:A:422:LEU:HG	1:A:423:VAL:N	2.21	0.51
1:A:511:ASP:O	1:A:522:ILE:HD13	2.10	0.51
2:B:79:GLU:CG	2:B:83:ARG:NH1	2.74	0.51
1:A:342:TYR:CD1	1:A:342:TYR:C	2.89	0.51
1:A:354:TYR:HD2	1:A:371:ALA:HB2	1.75	0.51
1:A:447:ASN:CB	1:A:450:THR:OG1	2.59	0.51
2:B:68:SER:O	2:B:69:THR:HG23	2.11	0.51
1:A:543:GLY:C	1:A:545:ASN:H	2.19	0.51
1:A:342:TYR:CD1	1:A:342:TYR:O	2.64	0.50
1:A:490:GLY:O	1:A:491:LEU:HD23	2.11	0.50
1:A:42:GLU:O	1:A:45:GLY:HA2	2.11	0.50
1:A:224:GLU:CB	1:A:225:PRO:CD	2.87	0.50
1:A:265:ASN:HD21	1:A:353:LYS:HZ2	1.59	0.50
1:A:419:THR:HG23	1:A:420:PRO:HD2	1.93	0.50
2:B:128:THR:CB	2:B:146:TYR:HB2	2.41	0.50
2:B:159:ILE:C	2:B:161:GLN:H	2.20	0.50
1:A:116:PHE:O	1:A:148:VAL:HG11	2.11	0.50
1:A:375:ILE:HG21	1:A:389:PHE:HZ	1.74	0.50
1:A:121:ASP:O	1:A:125:ARG:HG3	2.11	0.50
1:A:397:THR:HG21	1:A:425:LEU:H	1.77	0.50
1:A:59:PRO:O	1:A:75:VAL:HG13	2.11	0.50
1:A:87:PHE:C	2:B:55:PRO:HB3	2.37	0.50
1:A:340:GLN:HA	1:A:351:THR:HG22	1.92	0.50
1:A:544:GLY:HA2	2:B:284:ARG:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:MET:HE2	2:B:168:LEU:HD21	1.92	0.50
2:B:193:LEU:HD11	2:B:201:LYS:HG2	1.93	0.50
2:B:258:GLN:HE22	2:B:289:LEU:HD21	1.72	0.50
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.10	0.50
2:B:364:ASP:O	2:B:367:GLN:HB2	2.12	0.50
1:A:153:TRP:O	1:A:155:GLY:N	2.45	0.50
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.77	0.50
2:B:282:LEU:HD22	2:B:295:LEU:HA	1.93	0.50
1:A:373:GLN:O	1:A:376:THR:N	2.44	0.50
1:A:381:VAL:O	1:A:381:VAL:HG12	2.11	0.50
2:B:200:THR:O	2:B:202:ILE:N	2.44	0.50
2:B:224:GLU:HB3	2:B:226:PRO:HD2	1.94	0.50
2:B:326:ILE:HG12	2:B:388:LYS:HB3	1.93	0.50
2:B:376:THR:O	2:B:380:ILE:HG12	2.11	0.50
1:A:326:ILE:HG22	1:A:342:TYR:O	2.12	0.49
1:A:483:TYR:HE1	1:A:524:GLN:CD	2.18	0.49
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.47	0.49
1:A:9:PRO:CG	2:B:53:GLU:HG2	2.40	0.49
1:A:365:VAL:HG11	1:A:401:TRP:HB3	1.94	0.49
1:A:458:VAL:HA	1:A:463:ARG:O	2.11	0.49
2:B:54:ASN:C	2:B:54:ASN:OD1	2.55	0.49
2:B:200:THR:C	2:B:202:ILE:N	2.68	0.49
1:A:391:LEU:CD2	1:A:392:PRO:HD2	2.43	0.49
2:B:154:LYS:CE	2:B:184:MET:HE1	2.42	0.49
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.47	0.49
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.77	0.49
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.11	0.49
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.48	0.49
1:A:46:LYS:CG	1:A:148:VAL:HG21	2.42	0.49
1:A:56:TYR:H	1:A:56:TYR:HD1	1.58	0.49
1:A:219:LYS:O	1:A:221:HIS:N	2.45	0.49
1:A:508:ALA:C	1:A:509:GLN:HG2	2.37	0.49
2:B:102:LYS:HA	2:B:102:LYS:HE2	1.94	0.49
1:A:476:LYS:O	1:A:479:LEU:HB3	2.12	0.49
1:A:160:PHE:CD1	1:A:160:PHE:C	2.91	0.49
1:A:225:PRO:HG3	1:A:236:PRO:HG3	1.94	0.49
1:A:373:GLN:OE1	2:B:400:THR:HG21	2.12	0.49
2:B:34:LEU:HD21	2:B:62:ALA:HB2	1.95	0.49
1:A:43:LYS:C	1:A:45:GLY:N	2.71	0.49
2:B:277:ARG:O	2:B:280:SER:N	2.45	0.49
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:O	1:A:142:ILE:HD12	2.12	0.48
1:A:379:SER:CB	1:A:387:PRO:HD3	2.43	0.48
1:A:517:LEU:O	1:A:521:ILE:HG13	2.13	0.48
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.95	0.48
1:A:19:PRO:HD3	1:A:83:ARG:HD3	1.94	0.48
1:A:96:HIS:CE1	1:A:98:ALA:HB3	2.47	0.48
1:A:326:ILE:HG12	1:A:327:ALA:N	2.27	0.48
1:A:457:TYR:O	1:A:458:VAL:HG23	2.13	0.48
1:A:483:TYR:HE2	1:A:520:GLN:NE2	2.12	0.48
2:B:202:ILE:O	2:B:205:LEU:N	2.45	0.48
2:B:234:LEU:HD12	2:B:381:VAL:HG21	1.95	0.48
2:B:41:MET:HG3	2:B:46:LYS:HD2	1.95	0.48
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.47	0.48
1:A:120:LEU:HD13	1:A:149:LEU:HD23	1.95	0.48
2:B:210:LEU:HD12	2:B:215:THR:O	2.13	0.48
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.48	0.48
1:A:95:PRO:HB2	2:B:136:ASN:ND2	2.28	0.48
1:A:144:TYR:N	1:A:144:TYR:HD1	2.11	0.48
2:B:125:ARG:NE	2:B:147:ASN:HA	2.28	0.48
1:A:39:THR:HG22	1:A:40:GLU:N	2.28	0.48
1:A:265:ASN:ND2	1:A:353:LYS:NZ	2.60	0.48
2:B:32:LYS:O	2:B:35:VAL:HG23	2.14	0.48
2:B:126:LYS:HE3	2:B:127:TYR:CE1	2.48	0.48
2:B:193:LEU:HB3	2:B:197:GLN:HB2	1.96	0.48
2:B:402:TRP:C	2:B:404:GLU:N	2.70	0.48
1:A:373:GLN:C	1:A:375:ILE:N	2.68	0.48
1:A:379:SER:OG	1:A:387:PRO:CG	2.62	0.48
2:B:264:LEU:HD13	2:B:276:VAL:HG12	1.94	0.48
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.49	0.48
2:B:59:PRO:O	2:B:75:VAL:HG12	2.14	0.48
1:A:37:ILE:HG22	1:A:38:CYS:N	2.28	0.48
2:B:31:ILE:HG12	2:B:133:PRO:HG2	1.96	0.48
2:B:59:PRO:HB2	2:B:76:ASP:HB2	1.94	0.48
2:B:131:THR:CG2	2:B:132:ILE:N	2.77	0.48
2:B:160:PHE:O	2:B:161:GLN:C	2.55	0.48
2:B:319:TYR:CE2	2:B:383:TRP:HD1	2.31	0.48
1:A:252:TRP:H	1:A:252:TRP:HD1	1.62	0.48
1:A:298:GLU:OE1	1:A:298:GLU:HA	2.14	0.48
1:A:31:ILE:HD13	1:A:134:SER:HA	1.95	0.47
1:A:178:ILE:HD11	1:A:189:VAL:CG1	2.44	0.47
2:B:242:GLU:N	2:B:243:PRO:CD	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ASP:O	2:B:259:LYS:HB2	2.14	0.47
2:B:107:THR:OG1	2:B:198:HIS:CE1	2.64	0.47
2:B:159:ILE:O	2:B:161:GLN:N	2.48	0.47
1:A:483:TYR:CE1	1:A:524:GLN:CG	2.97	0.47
2:B:328:GLU:O	2:B:339:TYR:HA	2.14	0.47
2:B:368:LEU:HD23	2:B:398:TRP:CZ3	2.48	0.47
1:A:21:VAL:CG1	1:A:22:LYS:H	2.22	0.47
1:A:400:THR:C	1:A:402:TRP:H	2.23	0.47
1:A:473:THR:C	1:A:475:GLN:N	2.71	0.47
1:A:522:ILE:HG22	1:A:523:GLU:N	2.30	0.47
2:B:354:TYR:CE1	2:B:374:LYS:HD2	2.49	0.47
1:A:248:GLN:CG	1:A:249:LYS:N	2.77	0.47
1:A:532:TYR:CE1	1:A:533:LEU:O	2.67	0.47
2:B:402:TRP:C	2:B:404:GLU:H	2.22	0.47
1:A:101:LYS:HE2	1:A:321:PRO:HD3	1.95	0.47
2:B:325:LEU:HD21	2:B:349:LEU:HD13	1.96	0.47
1:A:246:LEU:HB3	1:A:263:LYS:HD2	1.96	0.47
1:A:473:THR:OG1	1:A:476:LYS:HB2	2.15	0.47
2:B:266:TRP:CE3	2:B:266:TRP:CA	2.96	0.47
1:A:227:PHE:O	1:A:234:LEU:HD12	2.15	0.47
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.98	0.47
1:A:391:LEU:HD23	1:A:392:PRO:HD2	1.97	0.47
1:A:552:VAL:HG12	1:A:552:VAL:O	2.15	0.47
2:B:224:GLU:HB2	2:B:228:LEU:HD12	1.96	0.47
2:B:329:ILE:HG22	2:B:330:GLN:H	1.78	0.47
2:B:375:ILE:O	2:B:378:GLU:HB2	2.15	0.47
1:A:342:TYR:HD1	1:A:342:TYR:C	2.23	0.47
1:A:522:ILE:O	1:A:525:LEU:HB2	2.15	0.47
2:B:43:LYS:O	2:B:45:GLY:N	2.47	0.47
2:B:369:THR:HA	2:B:398:TRP:CH2	2.47	0.47
1:A:229:TRP:O	1:A:230:MET:C	2.58	0.46
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.97	0.46
2:B:76:ASP:C	2:B:78:ARG:H	2.24	0.46
2:B:148:VAL:HG23	2:B:149:LEU:N	2.30	0.46
2:B:225:PRO:C	2:B:227:PHE:H	2.22	0.46
2:B:167:ILE:O	2:B:208:HIS:CE1	2.59	0.46
1:A:87:PHE:CE2	1:A:155:GLY:CA	2.98	0.46
1:A:153:TRP:HE3	1:A:156:SER:N	2.14	0.46
2:B:21:VAL:CG1	2:B:22:LYS:N	2.79	0.46
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.97	0.46
2:B:161:GLN:O	2:B:164:MET:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD13	2:B:296:THR:CG2	2.45	0.46
2:B:13:LYS:O	2:B:15:GLY:N	2.49	0.46
1:A:23:GLN:CD	1:A:60:VAL:H	2.24	0.46
1:A:74:LEU:CD1	1:A:75:VAL:H	2.25	0.46
1:A:486:LEU:HD11	1:A:521:ILE:HG23	1.97	0.46
2:B:184:MET:HG2	2:B:410:TRP:HD1	1.80	0.46
2:B:325:LEU:O	2:B:387:PRO:HA	2.16	0.46
2:B:424:LYS:O	2:B:426:TRP:N	2.48	0.46
1:A:8:VAL:O	1:A:121:ASP:HB2	2.16	0.46
1:A:90:VAL:O	1:A:92:LEU:N	2.48	0.46
1:A:323:LYS:O	1:A:343:GLN:NE2	2.49	0.46
1:A:400:THR:O	1:A:404:GLU:N	2.48	0.46
2:B:5:ILE:HG22	2:B:6:GLU:N	2.31	0.46
2:B:28:GLU:O	2:B:29:GLU:C	2.59	0.46
2:B:200:THR:C	2:B:202:ILE:H	2.23	0.46
2:B:260:LEU:O	2:B:260:LEU:HD12	2.16	0.46
2:B:369:THR:HG23	2:B:398:TRP:CH2	2.51	0.46
2:B:392:PRO:O	2:B:393:ILE:HB	2.15	0.46
1:A:201:LYS:HA	1:A:204:GLU:HB2	1.98	0.46
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.97	0.46
2:B:27:THR:HG22	2:B:29:GLU:H	1.81	0.46
2:B:124:PHE:CE2	2:B:153:TRP:CH2	3.03	0.46
2:B:115:TYR:N	2:B:115:TYR:HD1	2.14	0.46
2:B:216:THR:HA	2:B:217:PRO:HD3	1.86	0.46
2:B:120:LEU:HD11	2:B:124:PHE:CD2	2.51	0.46
1:A:326:ILE:HD11	1:A:390:LYS:HG2	1.97	0.45
1:A:363:ASN:HA	1:A:510:PRO:HA	1.98	0.45
2:B:183:TYR:CE2	2:B:380:ILE:HD12	2.51	0.45
2:B:346:PHE:HA	2:B:430:GLU:OXT	2.17	0.45
1:A:307:ARG:O	1:A:311:LYS:N	2.49	0.45
2:B:31:ILE:CG2	2:B:133:PRO:O	2.65	0.45
2:B:52:PRO:C	2:B:54:ASN:H	2.23	0.45
2:B:105:SER:O	2:B:198:HIS:NE2	2.49	0.45
1:A:79:GLU:HG2	1:A:83:ARG:NH1	2.31	0.45
1:A:79:GLU:O	1:A:83:ARG:HD2	2.15	0.45
2:B:116:PHE:HD1	2:B:148:VAL:CG2	2.30	0.45
2:B:398:TRP:C	2:B:400:THR:N	2.75	0.45
1:A:153:TRP:HB3	1:A:156:SER:OG	2.16	0.45
2:B:100:LEU:HG	2:B:381:VAL:O	2.16	0.45
2:B:238:LYS:HB2	2:B:239:TRP:CZ3	2.51	0.45
2:B:405:TYR:CD1	2:B:405:TYR:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:CG2	1:A:187:LEU:HD11	2.47	0.45
1:A:339:TYR:CD1	1:A:339:TYR:O	2.69	0.45
1:A:426:TRP:H	1:A:426:TRP:CD1	2.33	0.45
3:A:559:HBX:O2	3:A:559:HBX:H5	2.17	0.45
1:A:235:HIS:O	1:A:237:ASP:N	2.49	0.45
1:A:343:GLN:HG3	1:A:349:LEU:CD2	2.47	0.45
1:A:513:SER:O	1:A:519:ASN:ND2	2.49	0.45
2:B:23:GLN:HE21	2:B:26:LEU:HD21	1.76	0.45
2:B:115:TYR:OH	2:B:185:ASP:HA	2.17	0.45
1:A:465:LYS:O	1:A:466:VAL:HG23	2.17	0.45
1:A:466:VAL:CG1	1:A:467:VAL:N	2.79	0.45
2:B:99:GLY:O	2:B:102:LYS:HB2	2.17	0.45
2:B:184:MET:HG2	2:B:410:TRP:CD1	2.51	0.45
2:B:264:LEU:HB3	2:B:276:VAL:HG11	1.99	0.45
2:B:425:LEU:CD1	2:B:426:TRP:H	2.30	0.45
1:A:76:ASP:C	1:A:78:ARG:H	2.25	0.45
2:B:37:ILE:HG22	2:B:38:CYS:H	1.80	0.45
1:A:76:ASP:O	1:A:78:ARG:HG2	2.17	0.45
1:A:398:TRP:O	1:A:399:GLU:C	2.60	0.45
1:A:265:ASN:ND2	1:A:353:LYS:HZ2	2.15	0.45
1:A:127:TYR:C	1:A:129:ALA:H	2.25	0.44
1:A:176:PRO:HG2	1:A:177:ASP:H	1.81	0.44
1:A:218:ASP:HB3	1:A:222:GLN:CB	2.47	0.44
1:A:379:SER:HB3	1:A:387:PRO:HD3	1.99	0.44
2:B:210:LEU:HD12	2:B:210:LEU:HA	1.60	0.44
2:B:330:GLN:CG	2:B:338:THR:OG1	2.63	0.44
1:A:326:ILE:CG2	1:A:342:TYR:O	2.65	0.44
1:A:153:TRP:CE3	1:A:156:SER:N	2.85	0.44
1:A:444:GLY:O	1:A:445:ALA:HB2	2.17	0.44
1:A:492:GLU:O	1:A:492:GLU:HG3	2.17	0.44
2:B:34:LEU:HD21	2:B:61:PHE:O	2.18	0.44
2:B:80:LEU:HD23	2:B:153:TRP:CD1	2.52	0.44
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.72	0.44
1:A:96:HIS:ND1	1:A:98:ALA:HB3	2.33	0.44
2:B:21:VAL:HG12	2:B:22:LYS:H	1.82	0.44
1:A:40:GLU:C	1:A:43:LYS:HB2	2.43	0.44
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.60	0.44
2:B:277:ARG:C	2:B:279:LEU:H	2.26	0.44
1:A:210:LEU:HD22	1:A:215:THR:HA	2.00	0.44
1:A:440:PHE:N	1:A:440:PHE:CD1	2.86	0.44
1:A:96:HIS:HD1	1:A:98:ALA:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:N	1:A:452:LEU:O	2.50	0.44
2:B:60:VAL:CG1	2:B:73:LYS:HE3	2.48	0.44
1:A:229:TRP:CB	1:A:234:LEU:CD1	2.86	0.44
2:B:43:LYS:C	2:B:45:GLY:H	2.25	0.44
2:B:159:ILE:C	2:B:161:GLN:N	2.76	0.44
2:B:210:LEU:O	2:B:214:LEU:N	2.50	0.44
1:A:181:TYR:CD1	1:A:182:GLN:N	2.86	0.43
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.45	0.43
1:A:522:ILE:CG2	1:A:523:GLU:N	2.81	0.43
2:B:87:PHE:CZ	2:B:91:GLN:NE2	2.86	0.43
2:B:179:VAL:O	2:B:180:ILE:HG13	2.18	0.43
2:B:235:HIS:O	2:B:239:TRP:CZ3	2.71	0.43
2:B:329:ILE:CG2	2:B:330:GLN:N	2.80	0.43
1:A:170:PRO:O	1:A:174:GLN:N	2.49	0.43
1:A:99:GLY:CA	1:A:383:TRP:HE1	2.31	0.43
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.53	0.43
1:A:470:THR:O	1:A:472:THR:HG23	2.18	0.43
1:A:486:LEU:O	1:A:489:SER:OG	2.28	0.43
2:B:343:GLN:HE21	2:B:349:LEU:CD1	2.30	0.43
1:A:8:VAL:HG11	2:B:52:PRO:HG2	1.99	0.43
1:A:532:TYR:CD1	1:A:532:TYR:C	2.96	0.43
1:A:546:GLN:O	1:A:550:LYS:CB	2.66	0.43
2:B:63:ILE:CG2	2:B:64:LYS:N	2.80	0.43
2:B:109:LEU:HD22	2:B:206:ARG:HE	1.84	0.43
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.83	0.43
1:A:482:ILE:HG22	1:A:495:ILE:CD1	2.41	0.43
1:A:273:GLY:O	1:A:309:ILE:HD13	2.19	0.43
1:A:336:GLN:C	1:A:337:TRP:CD1	2.96	0.43
1:A:498:ASP:OD1	1:A:542:ILE:HG21	2.19	0.43
2:B:57:ASN:OD1	2:B:58:THR:N	2.47	0.43
2:B:81:ASN:C	2:B:83:ARG:N	2.76	0.43
2:B:120:LEU:HD23	2:B:125:ARG:CG	2.48	0.43
2:B:330:GLN:HE21	2:B:330:GLN:HB3	1.63	0.43
1:A:442:VAL:CG2	1:A:495:ILE:HG23	2.48	0.43
2:B:39:THR:O	2:B:42:GLU:HB3	2.19	0.43
1:A:136:ASN:O	1:A:138:GLU:N	2.52	0.43
1:A:543:GLY:C	1:A:545:ASN:N	2.74	0.43
2:B:94:ILE:HD11	2:B:158:ALA:HA	2.01	0.43
2:B:156:SER:O	2:B:158:ALA:N	2.50	0.43
2:B:227:PHE:CG	2:B:227:PHE:O	2.72	0.43
2:B:343:GLN:NE2	2:B:349:LEU:HD11	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:VAL:HB	2:B:91:GLN:H	1.54	0.43
2:B:422:LEU:O	2:B:425:LEU:HD23	2.18	0.43
1:A:446:ALA:HA	1:A:452:LEU:O	2.19	0.43
1:A:470:THR:HG22	1:A:471:ASN:N	2.34	0.43
2:B:213:GLY:O	2:B:214:LEU:C	2.61	0.43
2:B:354:TYR:CD1	2:B:374:LYS:HD2	2.53	0.43
1:A:229:TRP:NE1	3:A:559:HBV:H113	2.34	0.42
1:A:262:GLY:O	1:A:265:ASN:HB2	2.19	0.42
2:B:264:LEU:HD13	2:B:276:VAL:HG11	2.01	0.42
2:B:337:TRP:O	2:B:338:THR:HG23	2.19	0.42
2:B:343:GLN:HE21	2:B:349:LEU:HD11	1.83	0.42
2:B:26:LEU:CD1	2:B:133:PRO:HG3	2.49	0.42
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.49	0.42
1:A:317:VAL:HG22	1:A:318:TYR:H	1.84	0.42
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.54	0.42
2:B:205:LEU:O	2:B:205:LEU:HD12	2.18	0.42
1:A:74:LEU:HD12	1:A:75:VAL:N	2.27	0.42
1:A:106:VAL:CG1	1:A:107:THR:N	2.78	0.42
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.87	0.42
2:B:193:LEU:HB2	2:B:198:HIS:HB2	2.01	0.42
2:B:391:LEU:HB2	2:B:415:GLU:O	2.19	0.42
1:A:10:VAL:HG13	1:A:85:GLN:HG2	2.02	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.77	0.42
1:A:364:ASP:O	1:A:365:VAL:C	2.62	0.42
2:B:82:LYS:HD2	2:B:413:GLU:OE2	2.20	0.42
1:A:106:VAL:HG12	1:A:107:THR:N	2.33	0.42
1:A:156:SER:CB	1:A:157:PRO:HD3	2.36	0.42
1:A:406:TRP:CG	1:A:407:GLN:N	2.87	0.42
1:A:533:LEU:HD12	1:A:533:LEU:N	2.35	0.42
2:B:42:GLU:O	2:B:42:GLU:HG2	2.20	0.42
1:A:149:LEU:HD11	1:A:159:ILE:HG21	2.01	0.42
1:A:380:ILE:HG22	1:A:381:VAL:N	2.35	0.42
2:B:60:VAL:HG13	2:B:73:LYS:HE3	2.02	0.42
2:B:75:VAL:HG21	2:B:77:PHE:CE2	2.54	0.42
2:B:195:ILE:HD13	2:B:195:ILE:H	1.85	0.42
2:B:291:GLU:O	2:B:293:ILE:N	2.53	0.42
1:A:7:THR:HG21	1:A:121:ASP:HA	2.02	0.42
1:A:42:GLU:O	1:A:45:GLY:N	2.53	0.42
1:A:276:VAL:O	1:A:277:ARG:C	2.62	0.42
2:B:394:GLN:O	2:B:395:LYS:C	2.63	0.42
1:A:108:VAL:HG21	1:A:227:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:O	1:A:162:SER:N	2.53	0.41
1:A:309:ILE:C	1:A:311:LYS:N	2.77	0.41
1:A:398:TRP:C	1:A:400:THR:H	2.29	0.41
1:A:484:LEU:O	1:A:485:ALA:C	2.62	0.41
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.55	0.41
1:A:442:VAL:HG12	1:A:443:ASP:H	1.85	0.41
2:B:23:GLN:NE2	2:B:26:LEU:CD2	2.75	0.41
2:B:77:PHE:CE2	2:B:150:PRO:HB3	2.54	0.41
2:B:197:GLN:O	2:B:201:LYS:HE2	2.20	0.41
1:A:37:ILE:CG2	1:A:38:CYS:N	2.81	0.41
1:A:96:HIS:CE1	1:A:98:ALA:CB	3.03	0.41
1:A:102:LYS:HG2	1:A:318:TYR:HB2	2.02	0.41
1:A:374:LYS:O	1:A:378:GLU:HB2	2.21	0.41
1:A:427:TYR:CE2	1:A:509:GLN:HB3	2.54	0.41
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.86	0.41
1:A:125:ARG:NH1	1:A:147:ASN:HD22	2.18	0.41
2:B:52:PRO:C	2:B:54:ASN:N	2.79	0.41
2:B:63:ILE:CG2	2:B:64:LYS:H	2.29	0.41
1:A:153:TRP:O	1:A:154:LYS:C	2.63	0.41
1:A:163:SER:O	1:A:167:ILE:HG13	2.19	0.41
1:A:182:GLN:O	1:A:182:GLN:HG3	2.18	0.41
1:A:225:PRO:HB3	1:A:236:PRO:CD	2.50	0.41
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.51	0.41
1:A:532:TYR:HE1	1:A:534:ALA:HB2	1.84	0.41
2:B:224:GLU:C	2:B:226:PRO:HD2	2.46	0.41
2:B:300:GLU:OE1	2:B:303:LEU:HD23	2.20	0.41
1:A:54:ASN:O	1:A:143:ARG:NH2	2.53	0.41
1:A:90:VAL:HG23	1:A:91:GLN:N	2.36	0.41
1:A:132:ILE:HB	1:A:142:ILE:O	2.21	0.41
1:A:416:PHE:CE1	1:A:417:VAL:O	2.74	0.41
2:B:31:ILE:HD13	2:B:133:PRO:O	2.20	0.41
2:B:346:PHE:N	2:B:346:PHE:CD1	2.88	0.41
2:B:425:LEU:CG	2:B:426:TRP:H	2.33	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD2	1.76	0.41
1:A:99:GLY:HA2	1:A:319:TYR:HB2	2.03	0.41
1:A:149:LEU:HD11	1:A:159:ILE:CG2	2.51	0.41
1:A:203:GLU:OE1	1:A:203:GLU:HA	2.19	0.41
1:A:309:ILE:C	1:A:311:LYS:H	2.29	0.41
1:A:440:PHE:N	1:A:440:PHE:HD1	2.19	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.51	0.41
1:A:523:GLU:HA	1:A:526:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LYS:HG2	2:B:74:LEU:N	2.36	0.41
2:B:161:GLN:O	2:B:164:MET:HB3	2.20	0.41
1:A:87:PHE:CE2	1:A:155:GLY:HA3	2.56	0.41
1:A:447:ASN:C	1:A:449:GLU:H	2.29	0.41
1:A:537:PRO:O	1:A:542:ILE:HG23	2.20	0.41
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.86	0.41
2:B:183:TYR:CZ	2:B:184:MET:HE2	2.56	0.41
1:A:104:LYS:N	1:A:192:ASP:OD1	2.54	0.41
1:A:266:TRP:CZ2	1:A:269:GLN:NE2	2.86	0.41
1:A:375:ILE:O	1:A:376:THR:C	2.64	0.41
1:A:452:LEU:H	1:A:452:LEU:HG	1.63	0.41
2:B:31:ILE:O	2:B:31:ILE:HG22	2.20	0.41
2:B:206:ARG:O	2:B:209:LEU:HB2	2.20	0.41
2:B:337:TRP:HB2	2:B:354:TYR:HB3	2.02	0.41
2:B:367:GLN:O	2:B:371:ALA:HB2	2.21	0.41
2:B:373:GLN:O	2:B:374:LYS:C	2.63	0.41
1:A:1:PRO:HD3	1:A:44:GLU:HG2	2.01	0.41
2:B:193:LEU:HB3	2:B:197:GLN:CB	2.51	0.41
1:A:8:VAL:HG13	2:B:53:GLU:CG	2.51	0.40
1:A:39:THR:O	1:A:43:LYS:HD3	2.19	0.40
1:A:379:SER:OG	1:A:387:PRO:HG3	2.20	0.40
1:A:57:ASN:CG	1:A:58:THR:H	2.30	0.40
1:A:137:ASN:O	1:A:140:PRO:HD3	2.21	0.40
1:A:291:GLU:O	1:A:291:GLU:HG3	2.20	0.40
1:A:407:GLN:HG3	2:B:393:ILE:HA	2.02	0.40
1:A:515:SER:CB	1:A:518:VAL:HG23	2.51	0.40
2:B:24:TRP:O	2:B:26:LEU:HD23	2.22	0.40
2:B:110:ASP:O	2:B:112:GLY:N	2.52	0.40
2:B:236:PRO:HA	2:B:239:TRP:CZ2	2.57	0.40
2:B:386:THR:HA	2:B:387:PRO:HD3	1.82	0.40
2:B:402:TRP:O	2:B:404:GLU:N	2.54	0.40
1:A:156:SER:HB2	1:A:157:PRO:CD	2.43	0.40
1:A:246:LEU:HD11	1:A:264:LEU:HD21	2.02	0.40
1:A:411:ILE:HA	1:A:412:PRO:HD2	1.81	0.40
2:B:80:LEU:O	2:B:83:ARG:HB2	2.21	0.40
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.95	0.40
2:B:156:SER:C	2:B:158:ALA:N	2.79	0.40
2:B:380:ILE:O	2:B:384:GLY:N	2.55	0.40
2:B:394:GLN:HB3	2:B:397:THR:CB	2.51	0.40
1:A:155:GLY:O	1:A:158:ALA:N	2.52	0.40
2:B:31:ILE:HD13	2:B:133:PRO:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:O	2:B:44:GLU:HG3	2.20	0.40
2:B:132:ILE:CG2	2:B:133:PRO:HD2	2.51	0.40
2:B:258:GLN:NE2	2:B:289:LEU:CD2	2.81	0.40
2:B:363:ASN:OD1	2:B:363:ASN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	556/558 (100%)	407 (73%)	110 (20%)	39 (7%)	1	7
2	B	428/430 (100%)	324 (76%)	69 (16%)	35 (8%)	0	5
All	All	984/988 (100%)	731 (74%)	179 (18%)	74 (8%)	1	6

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	67	ASP
1	A	104	LYS
1	A	137	ASN
1	A	154	LYS
1	A	195	ILE
1	A	220	LYS
1	A	225	PRO
1	A	242	GLN
1	A	277	ARG
1	A	538	ALA
1	A	545	ASN
2	B	14	PRO
2	B	44	GLU

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Mol	Chain	Res	Type
2	B	85	GLN
2	B	125	ARG
2	B	153	TRP
2	B	212	TRP
2	B	244	ILE
2	B	311	LYS
2	B	317	VAL
2	B	425	LEU
1	A	153	TRP
1	A	284	ARG
1	A	286	THR
1	A	413	GLU
1	A	448	ARG
1	A	540	LYS
2	B	67	ASP
2	B	98	ALA
2	B	243	PRO
2	B	278	ALA
2	B	292	VAL
2	B	315	HIS
2	B	345	PRO
2	B	356	ARG
2	B	421	PRO
2	B	427	TYR
1	A	184	MET
1	A	217	PRO
1	A	218	ASP
1	A	240	THR
1	A	321	PRO
1	A	399	GLU
2	B	78	ARG
2	B	211	ARG
1	A	222	GLN
1	A	236	PRO
1	A	247	PRO
1	A	510	PRO
2	B	69	THR
2	B	260	LEU
2	B	316	GLY
2	B	362	THR
2	B	423	VAL
1	A	243	PRO

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Mol	Chain	Res	Type
1	A	374	LYS
1	A	436	GLY
2	B	138	GLU
2	B	160	PHE
2	B	213	GLY
1	A	63	ILE
1	A	91	GLN
1	A	156	SER
1	A	405	TYR
1	A	465	LYS
2	B	403	THR
1	A	548	VAL
2	B	381	VAL
1	A	359	GLY
2	B	169	GLU
2	B	242	GLU
1	A	176	PRO
2	B	159	ILE

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	455/498 (91%)	355 (78%)	100 (22%)	1	5
2	B	365/391 (93%)	292 (80%)	73 (20%)	1	6
All	All	820/889 (92%)	647 (79%)	173 (21%)	1	5

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	PRO
1	A	8	VAL
1	A	16	MET
1	A	20	LYS

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Mol	Chain	Res	Type
1	A	28	GLU
1	A	29	GLU
1	A	37	ILE
1	A	39	THR
1	A	41	MET
1	A	44	GLU
1	A	46	LYS
1	A	56	TYR
1	A	61	PHE
1	A	65	LYS
1	A	76	ASP
1	A	79	GLU
1	A	81	ASN
1	A	94	ILE
1	A	104	LYS
1	A	107	THR
1	A	108	VAL
1	A	111	VAL
1	A	122	GLU
1	A	126	LYS
1	A	135	ILE
1	A	144	TYR
1	A	146	TYR
1	A	154	LYS
1	A	168	LEU
1	A	182	GLN
1	A	187	LEU
1	A	197	GLN
1	A	210	LEU
1	A	211	ARG
1	A	214	LEU
1	A	216	THR
1	A	221	HIS
1	A	223	LYS
1	A	225	PRO
1	A	227	PHE
1	A	228	LEU
1	A	234	LEU
1	A	238	LYS
1	A	242	GLN
1	A	246	LEU
1	A	252	TRP

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	270	ILE
1	A	274	ILE
1	A	282	LEU
1	A	290	THR
1	A	291	GLU
1	A	295	LEU
1	A	296	THR
1	A	300	GLU
1	A	308	GLU
1	A	310	LEU
1	A	312	GLU
1	A	325	LEU
1	A	339	TYR
1	A	341	ILE
1	A	349	LEU
1	A	350	LYS
1	A	357	MET
1	A	362	THR
1	A	364	ASP
1	A	368	LEU
1	A	377	THR
1	A	379	SER
1	A	380	ILE
1	A	393	ILE
1	A	397	THR
1	A	403	THR
1	A	404	GLU
1	A	409	THR
1	A	423	VAL
1	A	428	GLN
1	A	429	LEU
1	A	431	LYS
1	A	440	PHE
1	A	442	VAL
1	A	450	THR
1	A	451	LYS
1	A	452	LEU
1	A	460	ASN
1	A	463	ARG
1	A	473	THR
1	A	478	GLU

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Mol	Chain	Res	Type
1	A	482	ILE
1	A	489	SER
1	A	497	THR
1	A	503	LEU
1	A	509	GLN
1	A	512	LYS
1	A	518	VAL
1	A	522	ILE
1	A	540	LYS
1	A	547	GLN
1	A	551	LEU
2	B	11	LYS
2	B	16	MET
2	B	26	LEU
2	B	32	LYS
2	B	35	VAL
2	B	37	ILE
2	B	47	ILE
2	B	50	ILE
2	B	53	GLU
2	B	59	PRO
2	B	63	ILE
2	B	65	LYS
2	B	67	ASP
2	B	74	LEU
2	B	75	VAL
2	B	85	GLN
2	B	86	ASP
2	B	92	LEU
2	B	100	LEU
2	B	104	LYS
2	B	105	SER
2	B	109	LEU
2	B	115	TYR
2	B	122	GLU
2	B	128	THR
2	B	132	ILE
2	B	139	THR
2	B	162	SER
2	B	163	SER
2	B	165	THR
2	B	166	LYS

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Mol	Chain	Res	Type
2	B	175	ASN
2	B	180	ILE
2	B	189	VAL
2	B	195	ILE
2	B	203	GLU
2	B	207	GLN
2	B	210	LEU
2	B	227	PHE
2	B	233	GLU
2	B	234	LEU
2	B	235	HIS
2	B	239	TRP
2	B	240	THR
2	B	242	GLU
2	B	252	TRP
2	B	253	THR
2	B	258	GLN
2	B	260	LEU
2	B	266	TRP
2	B	268	SER
2	B	270	ILE
2	B	290	THR
2	B	296	THR
2	B	324	ASP
2	B	330	GLN
2	B	331	LYS
2	B	332	GLN
2	B	341	ILE
2	B	345	PRO
2	B	350	LYS
2	B	356	ARG
2	B	358	ARG
2	B	362	THR
2	B	365	VAL
2	B	367	GLN
2	B	369	THR
2	B	380	ILE
2	B	400	THR
2	B	403	THR
2	B	409	THR
2	B	425	LEU
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	182	GLN
1	A	197	GLN
1	A	198	HIS
1	A	208	HIS
1	A	265	ASN
1	A	278	GLN
1	A	306	ASN
1	A	332	GLN
1	A	367	GLN
1	A	460	ASN
1	A	474	ASN
1	A	475	GLN
1	A	520	GLN
2	B	136	ASN
2	B	137	ASN
2	B	145	GLN
2	B	161	GLN
2	B	198	HIS
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	343	GLN
2	B	348	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	HBY	A	559	-	22,23,23	4.48	17 (77%)	24,32,32	1.70	4 (16%)

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	HBY	A	559	-	-	8/13/29/29	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	559	HBY	C9-N1	10.08	1.51	1.37
3	A	559	HBY	C3-C4	7.61	1.48	1.40
3	A	559	HBY	C2-S1	6.50	1.76	1.66
3	A	559	HBY	C1-N1	6.08	1.55	1.47
3	A	559	HBY	O2-C9	5.42	1.45	1.34
3	A	559	HBY	O1-C9	5.38	1.29	1.21
3	A	559	HBY	O3-C6	5.36	1.48	1.37
3	A	559	HBY	C2-N2	5.07	1.42	1.36
3	A	559	HBY	C13-S2	4.22	1.91	1.81
3	A	559	HBY	O2-C10	3.40	1.55	1.47
3	A	559	HBY	C5-C6	3.39	1.44	1.39
3	A	559	HBY	C7-C6	3.29	1.44	1.38
3	A	559	HBY	C8-C7	3.28	1.44	1.38
3	A	559	HBY	C13-C1	2.63	1.58	1.52
3	A	559	HBY	C4-N1	2.57	1.46	1.42
3	A	559	HBY	O3-C15	2.23	1.49	1.42
3	A	559	HBY	C3-N2	2.16	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	559	HBX	O2-C9-N1	4.09	116.34	110.93
3	A	559	HBX	C3-N2-C2	-3.97	121.34	124.76
3	A	559	HBX	C10-O2-C9	3.39	121.33	116.75
3	A	559	HBX	O1-C9-N1	-2.75	119.50	123.99

There are no chirality outliers.

All (8) torsion outliers are listed below:

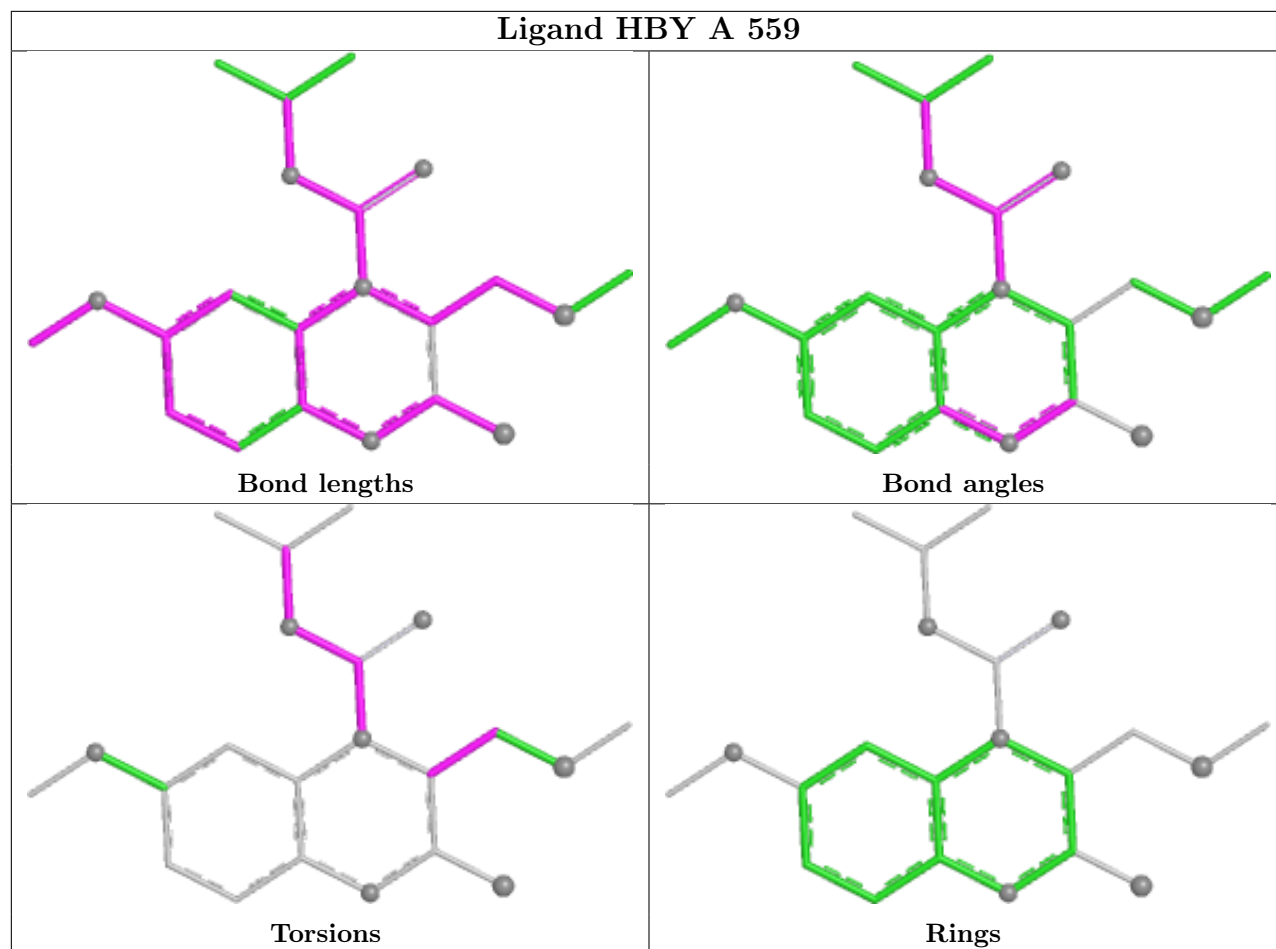
Mol	Chain	Res	Type	Atoms
3	A	559	HBX	C2-C1-C13-S2
3	A	559	HBX	N1-C1-C13-S2
3	A	559	HBX	N1-C9-O2-C10
3	A	559	HBX	O1-C9-O2-C10
3	A	559	HBX	C11-C10-O2-C9
3	A	559	HBX	O1-C9-N1-C4
3	A	559	HBX	C12-C10-O2-C9
3	A	559	HBX	O2-C9-N1-C4

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	559	HBX	8	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.