



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:39 AM UTC

PDB ID : 2JLE / pdb_00002jle
Title : Novel indazole nrtis created using molecular template hybridization based on crystallographic overlays
Authors : Jones, L.H.; Allan, G.; Barba, O.; Burt, C.; Corbau, R.; Dupont, T.; Irving, S.; Mowbray, C.E.; Phillips, C.; Swain, N.A.; Webster, R.; Westby, M.
Deposited on : 2008-09-08
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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

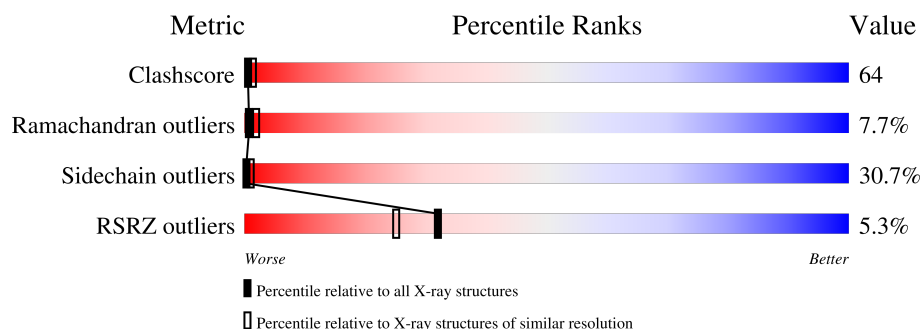
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	5% 18% 46% 26% 6%
1	B	566	4% 16% 33% 21% 27%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8120 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.

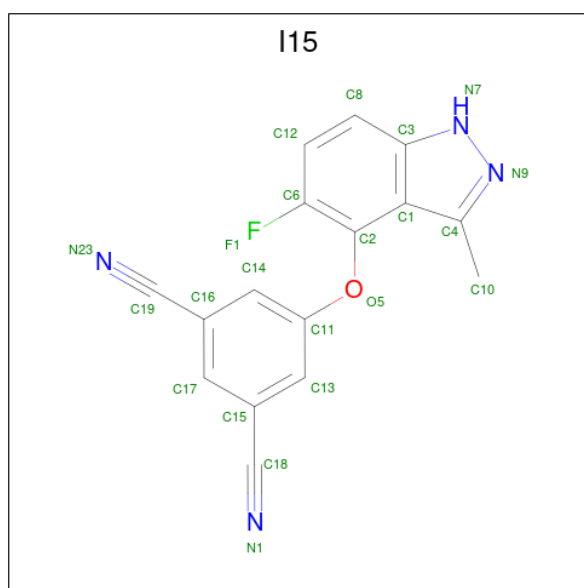
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RNASEH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4445	2875	742	820	8			
1	B	416	Total	C	N	O	S	0	0	1
			3414	2218	569	620	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	LYS	ARG	conflict	UNP Q72547
B	103	LYS	ARG	conflict	UNP Q72547
A	350	LYS	ARG	conflict	UNP Q72547
B	350	LYS	ARG	conflict	UNP Q72547

- Molecule 2 is 5-[(5-fluoro-3-methyl-1H-indazol-4-yl)oxy]benzene-1,3-dicarbonitrile (CCD ID: I15) (formula: C₁₆H₉FN₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			22	16	1	4	1		

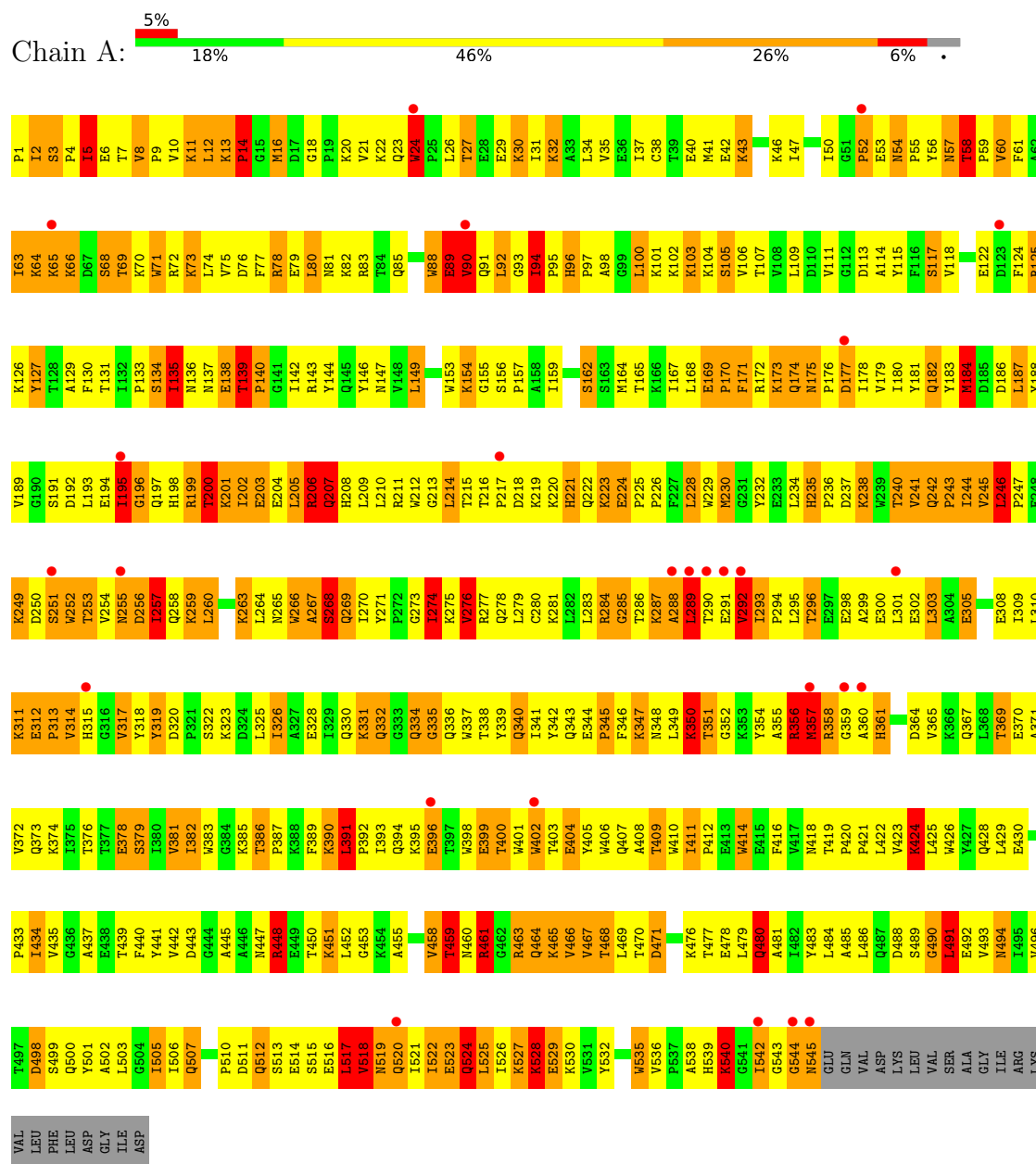
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	87	Total	O	0	0
			87	87		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: REVERSE TRANSCRIPTASE/RNASEH



• Molecule 1: REVERSE TRANSCRIPTASE/RNASEH



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.20Å 154.60Å 155.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.13 – 2.90 14.13 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (14.13-2.90) 89.7 (14.13-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.90Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.261 , 0.351 0.276 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 85.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I15

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.08	5/4562 (0.1%)	1.61	98/6199 (1.6%)
1	B	1.05	2/3510 (0.1%)	1.63	68/4772 (1.4%)
All	All	1.07	7/8072 (0.1%)	1.62	166/10971 (1.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	VAL	CA-CB	-8.13	1.45	1.54
1	A	346	PHE	N-CA	-6.64	1.37	1.46
1	A	518	VAL	CA-CB	-6.31	1.45	1.54
1	A	159	ILE	CA-CB	5.36	1.60	1.54
1	B	135	ILE	CA-CB	5.31	1.60	1.54
1	A	118	VAL	CA-CB	5.23	1.60	1.54
1	B	429	LEU	C-N	-5.08	1.26	1.33

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	GLU	CA-C-N	19.23	143.88	119.84
1	B	312	GLU	C-N-CA	19.23	143.88	119.84
1	B	320	ASP	CA-C-N	17.27	138.28	119.28
1	B	320	ASP	C-N-CA	17.27	138.28	119.28
1	A	224	GLU	CA-C-N	15.97	136.83	120.38
1	A	224	GLU	C-N-CA	15.97	136.83	120.38
1	A	13	LYS	CA-C-N	15.05	138.65	119.84
1	A	13	LYS	C-N-CA	15.05	138.65	119.84
1	A	8	VAL	CA-C-N	13.59	136.83	119.84
1	A	8	VAL	C-N-CA	13.59	136.83	119.84
1	B	94	ILE	CA-C-N	12.65	133.18	119.90
1	B	94	ILE	C-N-CA	12.65	133.18	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	PRO	CA-C-N	11.57	132.89	119.47
1	B	420	PRO	C-N-CA	11.57	132.89	119.47
1	A	246	LEU	CA-C-N	10.77	133.30	119.84
1	A	246	LEU	C-N-CA	10.77	133.30	119.84
1	B	3	SER	CA-C-N	10.15	132.53	119.84
1	B	3	SER	C-N-CA	10.15	132.53	119.84
1	A	410	TRP	N-CA-C	10.06	123.93	107.32
1	B	344	GLU	CA-C-N	9.83	132.13	119.84
1	B	344	GLU	C-N-CA	9.83	132.13	119.84
1	A	461	ARG	N-CA-C	-9.48	100.08	112.41
1	B	425	LEU	N-CA-C	8.97	120.99	111.03
1	B	58	THR	CA-C-N	-8.79	111.33	120.03
1	B	58	THR	C-N-CA	-8.79	111.33	120.03
1	B	195	ILE	N-CA-C	8.44	118.52	110.42
1	A	480	GLN	N-CA-C	-8.38	102.22	111.36
1	A	235	HIS	N-CA-C	-8.25	97.71	110.58
1	B	360	ALA	N-CA-C	-8.18	99.32	110.68
1	A	52	PRO	N-CA-C	-8.15	103.26	114.27
1	A	386	THR	CA-C-N	-8.08	109.74	119.84
1	A	386	THR	C-N-CA	-8.08	109.74	119.84
1	A	50	ILE	N-CA-C	8.04	122.25	108.90
1	A	358	ARG	N-CA-C	-7.97	104.06	113.38
1	A	414	TRP	N-CA-C	7.91	120.92	109.14
1	B	401	TRP	N-CA-C	7.85	123.03	113.38
1	A	500	GLN	N-CA-C	-7.82	102.76	111.28
1	A	357	MET	N-CA-C	-7.78	94.23	110.80
1	B	415	GLU	N-CA-C	-7.72	98.79	110.14
1	B	64	LYS	N-CA-C	7.69	120.72	110.88
1	A	54	ASN	CA-C-N	7.67	129.42	119.84
1	A	54	ASN	C-N-CA	7.67	129.42	119.84
1	A	242	GLN	CA-C-N	7.58	129.32	119.84
1	A	242	GLN	C-N-CA	7.58	129.32	119.84
1	B	194	GLU	N-CA-C	-7.50	100.43	110.55
1	A	114	ALA	N-CA-C	7.37	119.01	110.97
1	B	132	ILE	CA-C-N	7.37	129.05	119.84
1	B	132	ILE	C-N-CA	7.37	129.05	119.84
1	B	151	GLN	N-CA-C	-7.36	99.59	110.48
1	A	391	LEU	CA-C-N	7.34	129.01	119.84
1	A	391	LEU	C-N-CA	7.34	129.01	119.84
1	A	293	ILE	CA-C-N	7.31	127.58	119.90
1	A	293	ILE	C-N-CA	7.31	127.58	119.90
1	B	391	LEU	CA-C-N	7.28	128.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	LEU	C-N-CA	7.28	128.94	119.84
1	B	260	LEU	N-CA-C	-7.22	105.00	113.88
1	A	400	THR	N-CA-C	-7.21	103.50	111.36
1	A	350	LYS	N-CA-C	7.13	119.41	108.07
1	A	517	LEU	N-CA-C	-7.11	103.53	111.28
1	A	214	LEU	N-CA-C	7.07	120.30	108.20
1	B	323	LYS	N-CA-C	7.03	121.49	110.32
1	A	257	ILE	N-CA-C	-7.02	104.14	111.58
1	A	313	PRO	N-CA-C	6.91	122.07	111.15
1	A	58	THR	N-CA-C	-6.88	98.39	109.40
1	A	149	LEU	CA-C-N	-6.87	112.69	119.76
1	A	149	LEU	C-N-CA	-6.87	112.69	119.76
1	A	267	ALA	N-CA-C	-6.80	103.86	111.28
1	A	448	ARG	N-CA-C	6.76	118.30	111.07
1	A	147	ASN	N-CA-C	-6.75	104.75	114.12
1	B	286	THR	N-CA-C	-6.63	96.67	110.80
1	B	339	TYR	N-CA-C	6.63	120.08	108.75
1	A	292	VAL	CB-CA-C	6.61	120.19	111.33
1	B	104	LYS	N-CA-C	-6.59	104.50	112.54
1	A	58	THR	CA-C-N	6.58	126.56	119.78
1	A	58	THR	C-N-CA	6.58	126.56	119.78
1	B	105	SER	N-CA-C	6.47	119.03	108.55
1	A	260	LEU	N-CA-C	-6.46	104.16	111.14
1	B	128	THR	N-CA-C	6.38	120.08	112.93
1	B	139	THR	N-CA-C	-6.36	101.30	110.08
1	A	411	ILE	CA-C-N	-6.36	111.89	119.84
1	A	411	ILE	C-N-CA	-6.36	111.89	119.84
1	A	7	THR	N-CA-C	-6.29	100.67	110.42
1	B	420	PRO	C-N-CD	-6.28	99.27	125.00
1	B	142	ILE	N-CA-C	-6.23	98.01	107.73
1	A	139	THR	C-N-CD	-6.21	99.53	125.00
1	B	28	GLU	N-CA-C	-6.17	105.76	113.28
1	A	94	ILE	N-CA-C	6.15	114.60	107.89
1	A	184	MET	CB-CA-C	-6.12	108.91	117.23
1	A	266	TRP	N-CA-C	-6.09	103.38	111.24
1	A	200	THR	N-CA-C	-6.09	106.46	114.31
1	B	266	TRP	N-CA-C	6.05	117.54	111.07
1	B	203	GLU	N-CA-C	-6.01	104.65	111.14
1	A	263	LYS	N-CA-C	-6.00	104.74	111.28
1	B	312	GLU	C-N-CD	-6.00	100.40	125.00
1	B	356	ARG	N-CA-C	5.97	118.71	110.35
1	B	175	ASN	CA-C-N	5.97	125.67	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASN	C-N-CA	5.97	125.67	119.82
1	A	287	LYS	N-CA-C	-5.92	98.19	110.80
1	B	379	SER	N-CA-C	-5.92	104.91	111.36
1	A	8	VAL	N-CA-C	-5.90	101.09	108.05
1	B	31	ILE	N-CA-C	-5.88	105.01	110.53
1	A	24	TRP	CA-C-N	-5.87	113.92	119.85
1	A	24	TRP	C-N-CA	-5.87	113.92	119.85
1	A	90	VAL	N-CA-C	5.86	121.53	109.34
1	A	135	ILE	N-CA-C	5.81	121.43	109.34
1	A	343	GLN	N-CA-C	-5.77	106.16	113.43
1	B	39	THR	N-CA-C	-5.77	105.74	112.89
1	A	178	ILE	N-CA-C	5.71	116.52	108.36
1	A	532	TYR	N-CA-C	-5.68	100.44	109.76
1	A	346	PHE	CB-CA-C	5.67	121.71	110.42
1	B	249	LYS	N-CA-C	5.67	122.87	110.80
1	A	544	GLY	N-CA-C	-5.65	107.97	114.69
1	B	241	VAL	N-CA-C	5.64	121.08	109.34
1	B	85	GLN	N-CA-C	5.63	122.80	110.80
1	A	100	LEU	N-CA-C	-5.63	101.32	109.59
1	A	540	LYS	N-CA-C	-5.61	101.62	109.69
1	B	358	ARG	N-CA-C	5.60	122.73	110.80
1	B	71	TRP	N-CA-C	5.60	122.73	110.80
1	A	75	VAL	N-CA-C	5.60	116.01	108.17
1	A	382	ILE	N-CA-C	5.56	115.75	110.53
1	A	491	LEU	N-CA-C	5.53	122.57	110.80
1	A	535	TRP	N-CA-C	5.53	118.41	109.40
1	A	404	GLU	N-CA-C	5.52	119.18	112.23
1	B	357	MET	N-CA-C	-5.50	98.40	108.02
1	B	283	LEU	N-CA-C	5.49	119.97	113.16
1	B	414	TRP	N-CA-C	5.48	118.38	109.06
1	A	411	ILE	CB-CA-C	-5.48	105.63	111.00
1	B	300	GLU	N-CA-C	-5.46	105.88	112.54
1	B	293	ILE	CA-C-N	5.46	125.36	119.85
1	B	293	ILE	C-N-CA	5.46	125.36	119.85
1	B	333	GLY	N-CA-C	-5.46	103.88	112.61
1	B	113	ASP	N-CA-C	-5.45	106.58	113.18
1	A	268	SER	CA-C-N	5.45	129.81	120.72
1	A	268	SER	C-N-CA	5.45	129.81	120.72
1	A	349	LEU	N-CA-C	-5.42	105.53	111.82
1	A	171	PHE	N-CA-C	-5.42	104.25	111.24
1	A	94	ILE	CB-CA-C	5.40	116.14	110.37
1	A	240	THR	N-CA-C	-5.39	101.11	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLN	N-CA-C	5.38	119.10	112.54
1	A	182	GLN	CB-CA-C	-5.36	102.19	111.30
1	A	347	LYS	N-CA-C	-5.35	98.57	107.99
1	B	125	ARG	N-CA-C	5.31	122.11	110.80
1	B	420	PRO	N-CA-C	-5.30	104.24	110.70
1	A	467	VAL	N-CA-C	5.29	116.84	109.80
1	B	27	THR	N-CA-C	-5.26	103.94	110.41
1	B	43	LYS	N-CA-C	-5.25	106.14	112.54
1	B	189	VAL	N-CA-C	5.24	114.30	106.85
1	B	134	SER	N-CA-C	-5.24	101.68	109.96
1	A	127	TYR	N-CA-C	5.21	118.90	112.54
1	B	344	GLU	C-N-CD	-5.20	103.68	125.00
1	A	88	TRP	N-CA-C	5.20	117.20	109.25
1	A	154	LYS	N-CA-C	5.19	119.93	111.37
1	A	356	ARG	N-CA-C	5.17	121.81	110.80
1	A	289	LEU	N-CA-C	-5.16	105.66	111.28
1	A	424	LYS	N-CA-C	5.15	117.01	109.24
1	A	319	TYR	N-CA-C	5.14	118.50	110.32
1	A	96	HIS	N-CA-C	-5.14	103.22	110.31
1	A	252	TRP	N-CA-C	5.13	117.09	108.73
1	B	30	LYS	N-CA-C	-5.12	106.88	113.23
1	B	197	GLN	N-CA-C	-5.09	105.81	111.36
1	A	459	THR	N-CA-C	5.09	117.93	109.94
1	A	408	ALA	N-CA-C	-5.08	102.34	109.96
1	A	519	ASN	N-CA-C	5.03	116.85	111.36
1	A	16	MET	N-CA-C	5.03	121.50	110.80
1	A	348	ASN	CB-CA-C	-5.03	102.05	110.29
1	A	24	TRP	N-CA-C	-5.01	102.88	109.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4445	0	4493	642	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3414	0	3443	408	0
2	A	22	0	9	1	0
3	A	152	0	0	26	0
3	B	87	0	0	9	0
All	All	8120	0	7945	1020	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 64.

All (1020) 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:104:LYS:HB3	1:A:192:ASP:HA	1.20	1.18
1:B:103:LYS:HE3	1:B:179:VAL:HG21	1.24	1.15
1:A:64:LYS:HE3	1:A:69:THR:HA	1.22	1.10
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.14	1.07
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.33	1.06
1:B:84:THR:HG21	1:B:153:TRP:HE1	1.20	1.05
1:A:52:PRO:HD2	1:A:53:GLU:HG2	1.38	1.03
1:B:241:VAL:HG23	1:B:243:PRO:HD3	1.36	1.03
1:B:260:LEU:HG	1:B:264:LEU:HD12	1.42	1.02
1:A:288:ALA:CB	1:A:291:GLU:HB2	1.90	1.01
1:A:102:LYS:HE2	1:A:320:ASP:HB2	1.41	1.01
1:A:538:ALA:HA	1:A:545:ASN:HD21	1.23	1.00
1:B:194:GLU:HG3	1:B:197:GLN:HB2	1.42	1.00
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.25	0.99
1:A:64:LYS:HB3	1:A:65:LYS:HA	1.45	0.98
1:B:13:LYS:HB2	1:B:16:MET:HE3	1.45	0.98
1:A:101:LYS:HD3	1:A:103:LYS:HE2	1.47	0.97
1:A:94:ILE:HD12	1:A:95:PRO:HD2	1.46	0.96
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.45	0.95
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.47	0.95
1:A:540:LYS:HB3	1:A:542:ILE:HD12	1.49	0.94
1:B:354:TYR:HE1	1:B:357:MET:HE2	1.29	0.94
1:A:257:ILE:HG22	1:A:283:LEU:HD11	1.49	0.94
1:A:381:VAL:HG12	1:A:382:ILE:N	1.82	0.93
1:B:103:LYS:HE3	1:B:179:VAL:CG2	1.98	0.93
1:B:209:LEU:HD22	1:B:214:LEU:HD12	1.49	0.93
1:A:241:VAL:HG22	1:A:266:TRP:NE1	1.85	0.92
1:A:96:HIS:HD2	1:A:98:ALA:H	1.08	0.92
1:B:175:ASN:HD21	1:B:201:LYS:HE2	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:HD1	1:A:295:LEU:HD11	1.33	0.91
1:A:258:GLN:HG3	1:A:283:LEU:CD2	2.01	0.91
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.69	0.90
1:A:435:VAL:HA	1:B:290:THR:HG21	1.53	0.90
1:A:241:VAL:HG22	1:A:266:TRP:CD1	2.07	0.90
1:B:246:LEU:HD21	1:B:310:LEU:HD11	1.52	0.89
1:A:311:LYS:HE3	1:A:311:LYS:HA	1.51	0.89
1:B:84:THR:HG21	1:B:153:TRP:NE1	1.86	0.89
1:A:88:TRP:HD1	1:A:90:VAL:HG13	1.37	0.89
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.54	0.89
1:B:241:VAL:CG2	1:B:243:PRO:HD3	2.02	0.89
1:B:365:VAL:O	1:B:369:THR:HG23	1.73	0.88
1:A:356:ARG:HD2	1:A:359:GLY:HA3	1.56	0.88
1:A:172:ARG:HH12	1:A:182:GLN:HE21	1.22	0.88
1:A:174:GLN:HA	1:A:174:GLN:NE2	1.86	0.87
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.08	0.87
1:A:335:GLY:HA2	1:A:367:GLN:NE2	1.89	0.87
1:A:334:GLN:HE22	1:A:336:GLN:HE21	1.23	0.87
1:B:118:VAL:HG12	1:B:149:LEU:HG	1.55	0.87
1:A:64:LYS:CE	1:A:69:THR:HA	2.03	0.87
1:A:293:ILE:CG1	1:A:294:PRO:HD2	2.05	0.87
1:B:28:GLU:HB2	1:B:135:ILE:HD11	1.52	0.87
1:A:172:ARG:HH12	1:A:182:GLN:NE2	1.73	0.86
1:B:215:THR:HG22	1:B:217:PRO:CD	2.06	0.86
1:A:252:TRP:HB3	1:A:257:ILE:CD1	2.05	0.86
1:A:424:LYS:HE2	1:A:426:TRP:CZ2	2.10	0.86
1:A:224:GLU:HB2	1:A:225:PRO:HD2	1.57	0.86
1:B:183:TYR:CE2	1:B:184:MET:HE3	2.09	0.86
1:A:5:ILE:HD13	1:A:167:ILE:HG13	1.55	0.86
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.40	0.86
1:B:163:SER:O	1:B:167:ILE:HG13	1.74	0.86
1:A:189:VAL:HG11	1:A:202:ILE:HD11	1.58	0.86
1:B:284:ARG:HB3	1:B:284:ARG:NH2	1.91	0.85
1:A:104:LYS:CB	1:A:192:ASP:HA	2.04	0.85
1:B:257:ILE:HG22	1:B:283:LEU:HD11	1.58	0.85
1:A:335:GLY:HA3	1:A:356:ARG:CG	2.07	0.84
1:B:103:LYS:HG2	1:B:191:SER:N	1.92	0.84
1:A:335:GLY:HA3	1:A:356:ARG:HG2	1.59	0.84
1:A:96:HIS:CD2	1:A:98:ALA:H	1.94	0.84
1:B:258:GLN:HG3	1:B:283:LEU:HD22	1.60	0.84
1:B:341:ILE:HD11	1:B:375:ILE:HG23	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:TYR:CE1	1:B:357:MET:HE2	2.12	0.84
1:A:396:GLU:H	1:A:396:GLU:CD	1.85	0.83
1:A:357:MET:CE	1:A:360:ALA:HB3	2.08	0.83
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.58	0.83
1:A:325:LEU:C	1:A:326:ILE:HD13	2.04	0.83
1:A:395:LYS:HD3	1:A:414:TRP:CZ3	2.13	0.83
1:B:84:THR:HG22	1:B:88:TRP:HD1	1.43	0.83
1:B:260:LEU:HG	1:B:264:LEU:CD1	2.08	0.83
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.61	0.83
1:A:402:TRP:CD1	1:A:403:THR:HG23	2.13	0.82
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.08	0.82
1:A:125:ARG:HG2	1:A:146:TYR:O	1.78	0.82
1:B:366:LYS:HG2	1:B:405:TYR:CD2	2.15	0.82
1:A:242:GLN:HG3	1:A:243:PRO:HD2	1.60	0.82
1:B:37:ILE:O	1:B:41:MET:HG3	1.80	0.82
1:B:215:THR:HG22	1:B:217:PRO:HD3	1.61	0.81
1:B:76:ASP:OD1	1:B:78:ARG:HG3	1.80	0.81
1:A:238:LYS:HE3	1:A:315:HIS:CG	2.15	0.81
1:B:28:GLU:CB	1:B:135:ILE:HD11	2.09	0.81
1:B:254:VAL:HB	1:B:289:LEU:HA	1.63	0.81
1:A:434:ILE:HG13	1:A:494:ASN:HD21	1.44	0.81
1:A:451:LYS:HB3	1:A:451:LYS:NZ	1.95	0.81
1:A:538:ALA:HA	1:A:545:ASN:ND2	1.94	0.81
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.15	0.81
1:A:516:GLU:O	1:A:520:GLN:HG2	1.80	0.81
1:B:91:GLN:C	1:B:92:LEU:HD23	2.06	0.81
1:A:258:GLN:HG3	1:A:283:LEU:HD21	1.63	0.80
1:A:424:LYS:HE2	1:A:426:TRP:CH2	2.15	0.80
1:B:81:ASN:ND2	1:B:154:LYS:HD2	1.97	0.80
1:B:175:ASN:ND2	1:B:201:LYS:HE2	1.96	0.80
1:A:486:LEU:HD22	1:A:528:LYS:HD2	1.63	0.80
1:A:350:LYS:HE3	1:A:378:GLU:OE2	1.81	0.79
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.64	0.79
1:B:3:SER:N	1:B:4:PRO:HD2	1.96	0.79
1:B:249:LYS:HD3	1:B:250:ASP:N	1.96	0.79
1:A:406:TRP:H	1:A:406:TRP:CD1	1.99	0.79
1:B:276:VAL:O	1:B:280:CYS:HB2	1.82	0.79
1:B:358:ARG:HB3	1:B:358:ARG:CZ	2.11	0.79
1:B:246:LEU:HD21	1:B:310:LEU:CD1	2.11	0.79
1:A:197:GLN:O	1:A:201:LYS:HB2	1.84	0.78
1:A:211:ARG:HD2	3:A:2070:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HG21	1:A:209:LEU:HD23	1.65	0.78
1:B:231:GLY:HA3	1:B:232:TYR:C	2.09	0.78
1:B:276:VAL:HA	1:B:302:GLU:OE2	1.84	0.77
1:A:357:MET:HE1	1:A:360:ALA:HB3	1.66	0.77
1:A:29:GLU:HG2	1:A:71:TRP:HH2	1.49	0.77
1:B:284:ARG:HB3	1:B:284:ARG:HH21	1.48	0.77
1:B:356:ARG:NH1	1:B:358:ARG:NH2	2.33	0.77
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.15	0.77
1:A:31:ILE:HD13	1:A:133:PRO:O	1.84	0.77
1:A:177:ASP:HB2	3:A:2059:HOH:O	1.85	0.77
1:B:278:GLN:HB2	1:B:302:GLU:OE1	1.85	0.77
1:A:21:VAL:HG12	1:A:59:PRO:HD3	1.67	0.77
1:A:538:ALA:CA	1:A:545:ASN:HD21	1.98	0.76
1:A:195:ILE:HG22	1:A:199:ARG:HD2	1.67	0.76
1:A:64:LYS:CB	1:A:65:LYS:HA	2.16	0.76
1:B:64:LYS:HE3	1:B:69:THR:OG1	1.85	0.76
1:A:206:ARG:HH21	1:A:218:ASP:N	1.83	0.76
1:A:545:ASN:HA	3:A:2139:HOH:O	1.86	0.76
1:A:228:LEU:HD13	1:A:242:GLN:HE21	1.50	0.76
1:A:419:THR:HG23	1:A:419:THR:O	1.86	0.76
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.82	0.75
1:B:249:LYS:HA	1:B:252:TRP:CZ2	2.20	0.75
1:A:311:LYS:HA	1:A:311:LYS:CE	2.14	0.75
1:A:516:GLU:HA	1:A:519:ASN:HB2	1.68	0.75
1:B:260:LEU:O	1:B:264:LEU:HD12	1.87	0.75
1:B:183:TYR:HE2	1:B:184:MET:HE3	1.49	0.75
1:A:29:GLU:HG2	1:A:71:TRP:CH2	2.21	0.74
1:B:27:THR:OG1	1:B:30:LYS:HG3	1.86	0.74
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.02	0.74
1:B:40:GLU:O	1:B:44:GLU:HG3	1.86	0.74
1:A:228:LEU:HD13	1:A:242:GLN:NE2	2.02	0.74
1:B:94:ILE:N	1:B:94:ILE:HD12	2.02	0.74
1:A:458:VAL:HG23	1:B:286:THR:CG2	2.17	0.74
1:B:21:VAL:CG2	1:B:79:GLU:HG3	2.18	0.74
1:A:394:GLN:HB3	1:A:396:GLU:OE1	1.86	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.87	0.74
1:A:258:GLN:HG3	1:A:283:LEU:HD22	1.69	0.74
1:A:101:LYS:HD3	1:A:103:LYS:CE	2.17	0.74
1:B:189:VAL:HB	1:B:202:ILE:HD11	1.70	0.73
1:B:253:THR:O	1:B:257:ILE:HG13	1.87	0.73
1:B:255:ASN:O	1:B:259:LYS:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HG3	1:B:255:ASN:ND2	2.04	0.73
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.54	0.73
1:B:66:LYS:HG3	1:B:407:GLN:OE1	1.88	0.73
1:A:247:PRO:HG2	3:A:2088:HOH:O	1.89	0.73
1:A:296:THR:CG2	1:A:299:ALA:H	2.02	0.73
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.24	0.72
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.71	0.72
1:A:173:LYS:HE3	1:A:174:GLN:HG2	1.70	0.72
1:A:510:PRO:HG3	3:A:2141:HOH:O	1.90	0.72
1:A:511:ASP:OD1	1:A:512:GLN:HG3	1.88	0.72
1:A:485:ALA:O	1:A:489:SER:HB3	1.89	0.72
1:A:88:TRP:CD1	1:A:90:VAL:HG13	2.24	0.72
1:B:312:GLU:OE1	1:B:313:PRO:HD2	1.89	0.72
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.72	0.71
1:B:20:LYS:HE3	1:B:55:PRO:HB2	1.72	0.71
1:A:271:TYR:CD1	1:A:310:LEU:HD23	2.24	0.71
1:B:345:PRO:O	1:B:346:PHE:HB2	1.89	0.71
1:A:406:TRP:HZ3	1:B:418:ASN:HA	1.56	0.71
1:A:491:LEU:H	1:A:491:LEU:HD23	1.55	0.71
1:B:371:ALA:O	1:B:375:ILE:HD12	1.90	0.71
1:B:162:SER:O	1:B:166:LYS:HD2	1.90	0.70
1:B:66:LYS:HA	1:B:407:GLN:NE2	2.05	0.70
1:B:134:SER:HB3	1:B:139:THR:HB	1.73	0.70
1:A:402:TRP:HD1	1:A:403:THR:HG23	1.57	0.70
1:A:524:GLN:O	1:A:526:ILE:N	2.25	0.70
1:B:269:GLN:HG2	1:B:346:PHE:CE2	2.26	0.70
1:B:331:LYS:HE3	1:B:364:ASP:OD2	1.89	0.70
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.17	0.70
1:B:85:GLN:HA	1:B:88:TRP:NE1	2.06	0.70
1:A:220:LYS:HB3	1:A:221:HIS:CD2	2.26	0.70
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.72	0.70
1:A:494:ASN:N	1:A:494:ASN:HD22	1.88	0.70
1:B:40:GLU:HG3	3:B:2015:HOH:O	1.90	0.70
1:B:284:ARG:O	1:B:284:ARG:HG2	1.91	0.70
1:B:248:GLU:HA	1:B:307:ARG:HH22	1.56	0.70
1:A:27:THR:HG22	1:A:29:GLU:HB3	1.73	0.69
1:A:355:ALA:O	1:A:356:ARG:O	2.10	0.69
1:A:390:LYS:C	1:A:391:LEU:HD23	2.16	0.69
1:A:434:ILE:HG13	1:A:494:ASN:ND2	2.07	0.69
1:A:53:GLU:O	1:A:55:PRO:HD3	1.93	0.69
1:A:461:ARG:HH11	1:A:461:ARG:CG	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:O	1:A:545:ASN:HB3	1.91	0.69
1:B:319:TYR:OH	1:B:385:LYS:HE3	1.92	0.69
1:A:536:VAL:HG21	1:A:545:ASN:HB2	1.75	0.69
1:B:72:ARG:NH2	1:B:151:GLN:HE22	1.91	0.69
1:A:245:VAL:O	1:A:247:PRO:HD3	1.92	0.69
1:B:92:LEU:HD23	1:B:92:LEU:N	2.08	0.69
1:A:58:THR:HG22	1:A:76:ASP:O	1.92	0.69
1:A:334:GLN:NE2	1:A:336:GLN:HE21	1.90	0.69
1:A:5:ILE:HD13	1:A:167:ILE:CG1	2.23	0.68
1:A:61:PHE:HB2	3:A:2025:HOH:O	1.91	0.68
1:A:277:ARG:NH2	1:A:334:GLN:HG3	2.07	0.68
1:A:464:GLN:HG3	1:A:465:LYS:N	2.08	0.68
1:B:182:GLN:HB2	1:B:187:LEU:HD23	1.74	0.68
1:B:103:LYS:HG2	1:B:190:GLY:C	2.19	0.68
1:B:72:ARG:HG2	1:B:73:LYS:N	2.09	0.68
1:B:122:GLU:CD	1:B:122:GLU:H	2.02	0.68
1:B:231:GLY:HA3	1:B:232:TYR:O	1.94	0.68
1:A:1:PRO:O	1:A:2:ILE:HG13	1.94	0.68
1:B:395:LYS:HG2	1:B:416:PHE:CE2	2.28	0.68
1:A:26:LEU:HD12	1:A:133:PRO:CD	2.24	0.67
1:A:164:MET:HE3	1:A:187:LEU:HD22	1.76	0.67
1:A:172:ARG:NH1	1:A:182:GLN:HE21	1.92	0.67
1:A:260:LEU:O	1:A:264:LEU:HB2	1.94	0.67
1:A:274:ILE:HD12	1:A:309:ILE:HG21	1.75	0.67
1:A:326:ILE:HD13	1:A:326:ILE:N	2.07	0.67
1:A:476:LYS:NZ	3:A:2138:HOH:O	2.28	0.67
1:A:216:THR:HG22	1:A:217:PRO:N	2.10	0.67
1:B:139:THR:HG22	1:B:140:PRO:O	1.94	0.67
1:A:37:ILE:CG2	1:A:41:MET:HE3	2.25	0.67
1:A:206:ARG:HH21	1:A:217:PRO:C	2.02	0.67
1:B:313:PRO:O	1:B:315:HIS:N	2.27	0.67
1:B:21:VAL:HB	1:B:59:PRO:HD3	1.77	0.67
1:B:274:ILE:C	1:B:275:LYS:HG2	2.20	0.67
1:B:241:VAL:HG23	1:B:243:PRO:CD	2.20	0.66
1:A:189:VAL:CG1	1:A:202:ILE:HD11	2.24	0.66
1:A:23:GLN:HE22	1:A:60:VAL:H	1.42	0.66
1:A:175:ASN:H	1:A:176:PRO:HD3	1.60	0.66
1:A:206:ARG:O	1:A:209:LEU:N	2.27	0.66
1:A:175:ASN:N	1:A:176:PRO:HD3	2.08	0.66
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.78	0.66
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:O	1:A:332:GLN:NE2	2.28	0.66
1:A:64:LYS:HE3	1:A:69:THR:CA	2.13	0.66
1:B:175:ASN:HB2	1:B:178:ILE:HG13	1.78	0.66
1:A:257:ILE:CG2	1:A:283:LEU:HD11	2.25	0.66
1:A:491:LEU:HD23	1:A:491:LEU:N	2.10	0.66
1:A:27:THR:HB	1:A:30:LYS:HD2	1.77	0.65
1:A:543:GLY:HA3	1:B:285:GLY:H	1.61	0.65
1:B:84:THR:CG2	1:B:153:TRP:HE1	2.04	0.65
1:A:101:LYS:CD	1:A:103:LYS:HE2	2.24	0.65
1:A:407:GLN:NE2	1:B:418:ASN:OD1	2.29	0.65
1:A:447:ASN:HB3	1:A:450:THR:OG1	1.95	0.65
1:A:96:HIS:HD2	1:A:98:ALA:N	1.89	0.65
1:B:295:LEU:H	1:B:295:LEU:HD12	1.62	0.65
1:B:114:ALA:HB1	1:B:160:PHE:CZ	2.32	0.65
1:B:341:ILE:HD11	1:B:375:ILE:CG2	2.27	0.65
1:A:458:VAL:HG23	1:B:286:THR:HG21	1.78	0.64
1:B:13:LYS:CB	1:B:16:MET:HE3	2.24	0.64
1:B:84:THR:HG22	1:B:88:TRP:CD1	2.28	0.64
1:A:103:LYS:NZ	1:A:192:ASP:OD2	2.30	0.64
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.78	0.64
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.79	0.64
1:B:214:LEU:N	1:B:214:LEU:HD23	2.12	0.64
1:A:275:LYS:HE3	1:A:305:GLU:OE1	1.97	0.64
1:B:278:GLN:N	1:B:302:GLU:OE1	2.30	0.64
1:A:335:GLY:CA	1:A:367:GLN:HE22	2.06	0.64
1:A:356:ARG:HH11	1:A:512:GLN:NE2	1.96	0.64
1:B:278:GLN:HG3	1:B:298:GLU:C	2.23	0.64
1:B:295:LEU:HD22	1:B:300:GLU:CD	2.23	0.64
1:A:11:LYS:HG3	1:A:12:LEU:N	2.12	0.63
1:B:142:ILE:HG22	1:B:144:TYR:CE1	2.34	0.63
1:A:52:PRO:CD	1:A:53:GLU:H	2.11	0.63
1:A:29:GLU:CG	1:A:71:TRP:HH2	2.11	0.63
1:A:172:ARG:NH1	1:A:182:GLN:NE2	2.46	0.63
1:B:28:GLU:OE2	1:B:32:LYS:NZ	2.29	0.63
1:A:228:LEU:HB3	1:A:242:GLN:HE22	1.63	0.63
1:A:293:ILE:HG12	1:A:294:PRO:HD2	1.80	0.63
1:B:279:LEU:HG	1:B:302:GLU:OE2	1.99	0.63
1:A:32:LYS:HD3	3:A:2016:HOH:O	1.97	0.63
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.28	0.63
1:A:271:TYR:CE1	1:A:310:LEU:HD23	2.33	0.63
1:A:334:GLN:NE2	1:A:334:GLN:O	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:N	1:B:283:LEU:O	2.27	0.63
1:B:94:ILE:HD12	1:B:94:ILE:H	1.64	0.63
1:B:12:LEU:HD11	1:B:127:TYR:CE1	2.34	0.63
1:B:360:ALA:CB	1:B:366:LYS:HZ3	2.11	0.63
1:B:21:VAL:HG21	1:B:79:GLU:HG3	1.80	0.62
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.81	0.62
1:B:114:ALA:HB2	1:B:214:LEU:HD13	1.81	0.62
1:A:97:PRO:HG2	1:A:232:TYR:CE2	2.34	0.62
1:A:503:LEU:HD23	1:B:422:LEU:HD11	1.80	0.62
1:B:319:TYR:O	1:B:321:PRO:HD3	1.99	0.62
1:A:13:LYS:O	1:A:16:MET:HB2	2.00	0.62
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.34	0.62
1:A:493:VAL:C	1:A:494:ASN:HD22	2.08	0.62
1:B:344:GLU:O	1:B:347:LYS:HB2	1.99	0.62
1:A:360:ALA:HB2	1:A:514:GLU:OE2	2.00	0.62
1:B:279:LEU:HA	1:B:282:LEU:CD1	2.29	0.62
1:A:162:SER:OG	1:B:52:PRO:HG3	2.00	0.62
1:A:460:ASN:ND2	1:B:288:ALA:HB2	2.14	0.62
1:B:85:GLN:O	1:B:85:GLN:HG3	1.98	0.62
1:A:252:TRP:HB3	1:A:257:ILE:HD12	1.81	0.62
1:A:253:THR:HA	1:A:292:VAL:HA	1.82	0.62
1:A:254:VAL:CG2	1:A:291:GLU:HB3	2.30	0.62
1:B:34:LEU:HD22	1:B:73:LYS:HG2	1.81	0.62
1:B:308:GLU:O	1:B:311:LYS:HD3	2.00	0.62
1:B:366:LYS:O	1:B:370:GLU:HG2	2.00	0.62
1:B:114:ALA:HB1	1:B:160:PHE:CE2	2.35	0.61
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.35	0.61
1:A:434:ILE:HD13	1:A:530:LYS:CB	2.25	0.61
1:B:20:LYS:HG2	1:B:55:PRO:O	2.00	0.61
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.32	0.61
1:B:210:LEU:HD12	1:B:210:LEU:O	1.99	0.61
1:A:199:ARG:O	1:A:219:LYS:NZ	2.30	0.61
1:A:1:PRO:O	1:A:46:LYS:NZ	2.33	0.61
1:B:203:GLU:O	1:B:206:ARG:HB2	2.01	0.61
1:A:303:LEU:HD12	1:A:303:LEU:O	2.01	0.61
1:B:215:THR:HG22	1:B:217:PRO:HD2	1.81	0.61
1:A:312:GLU:OE2	1:A:312:GLU:N	2.27	0.61
1:B:387:PRO:HG2	1:B:389:PHE:CZ	2.36	0.61
1:B:324:ASP:O	1:B:343:GLN:HG2	2.01	0.60
1:A:93:GLY:O	1:B:137:ASN:ND2	2.34	0.60
1:B:118:VAL:CG1	1:B:149:LEU:HG	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TRP:H	1:A:71:TRP:CD1	2.19	0.60
1:A:335:GLY:CA	1:A:356:ARG:HG2	2.30	0.60
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.36	0.60
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.83	0.60
1:B:374:LYS:O	1:B:378:GLU:HG3	2.01	0.60
1:B:425:LEU:O	1:B:428:GLN:HB3	2.01	0.60
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.84	0.60
1:B:379:SER:HB2	1:B:385:LYS:O	2.02	0.60
1:B:258:GLN:HG3	1:B:283:LEU:CD2	2.31	0.60
1:B:395:LYS:HD3	1:B:399:GLU:CD	2.27	0.60
1:A:194:GLU:O	1:A:196:GLY:N	2.34	0.60
1:A:228:LEU:HB3	1:A:242:GLN:NE2	2.17	0.60
1:A:210:LEU:C	1:A:212:TRP:H	2.07	0.60
1:B:92:LEU:HB2	1:B:158:ALA:HB1	1.82	0.60
1:A:238:LYS:HE3	1:A:315:HIS:CD2	2.37	0.59
1:A:242:GLN:CG	1:A:243:PRO:HD2	2.30	0.59
1:A:296:THR:HG22	1:A:299:ALA:H	1.65	0.59
1:A:369:THR:O	1:A:373:GLN:HB2	2.02	0.59
1:B:241:VAL:HG23	1:B:242:GLN:N	2.16	0.59
1:A:167:ILE:CG2	1:A:209:LEU:HD23	2.33	0.59
1:A:206:ARG:NH2	1:A:218:ASP:OD1	2.35	0.59
1:A:252:TRP:CB	1:A:257:ILE:HD11	2.30	0.59
1:A:398:TRP:CH2	1:A:409:THR:HG23	2.37	0.59
1:B:13:LYS:HE3	1:B:16:MET:HE1	1.83	0.59
1:B:376:THR:CG2	1:B:386:THR:HG22	2.32	0.59
1:A:37:ILE:HG23	1:A:41:MET:HE3	1.83	0.59
1:A:241:VAL:CG2	1:A:266:TRP:CD1	2.85	0.59
1:B:254:VAL:HG23	1:B:291:GLU:O	2.02	0.59
1:B:248:GLU:HA	1:B:307:ARG:NH2	2.17	0.59
1:A:543:GLY:HA3	1:B:285:GLY:N	2.17	0.59
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.18	0.59
1:A:30:LYS:HD3	3:A:2011:HOH:O	2.03	0.58
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.18	0.58
1:A:460:ASN:HA	1:B:286:THR:O	2.02	0.58
1:A:527:LYS:O	1:A:528:LYS:O	2.21	0.58
1:B:351:THR:O	1:B:351:THR:OG1	2.20	0.58
1:A:254:VAL:HG23	1:A:291:GLU:O	2.03	0.58
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.39	0.58
1:B:34:LEU:CD2	1:B:73:LYS:HG2	2.33	0.58
1:B:78:ARG:NH1	1:B:412:PRO:O	2.36	0.58
1:B:216:THR:H	1:B:217:PRO:CD	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PRO:HG2	1:B:389:PHE:CE1	2.38	0.58
1:A:189:VAL:HG11	1:A:202:ILE:CD1	2.33	0.58
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.84	0.58
1:A:265:ASN:HA	1:A:268:SER:HB3	1.85	0.58
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.32	0.58
1:A:155:GLY:HA2	3:A:2053:HOH:O	2.04	0.58
1:A:172:ARG:NH2	1:A:180:ILE:O	2.37	0.58
1:B:272:PRO:O	1:B:274:ILE:N	2.37	0.58
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.32	0.58
1:A:93:GLY:C	1:B:137:ASN:HD22	2.12	0.58
1:B:103:LYS:HD3	1:B:190:GLY:HA3	1.86	0.58
1:B:278:GLN:NE2	1:B:298:GLU:HB2	2.18	0.58
1:B:30:LYS:HB3	1:B:62:ALA:HB3	1.84	0.58
1:B:50:ILE:CG2	1:B:145:GLN:HB3	2.33	0.58
1:A:198:HIS:C	1:A:200:THR:H	2.12	0.57
1:A:221:HIS:CD2	1:A:221:HIS:N	2.71	0.57
1:A:285:GLY:HA2	1:A:286:THR:OG1	2.03	0.57
1:B:295:LEU:HD13	1:B:300:GLU:OE2	2.04	0.57
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.03	0.57
1:B:72:ARG:HH21	1:B:151:GLN:NE2	2.02	0.57
1:B:249:LYS:HA	1:B:252:TRP:HZ2	1.67	0.57
1:B:335:GLY:HA3	1:B:356:ARG:HB3	1.85	0.57
1:A:295:LEU:HD12	1:A:295:LEU:H	1.69	0.57
1:A:511:ASP:C	1:A:512:GLN:HG3	2.29	0.57
1:B:422:LEU:HB3	1:B:426:TRP:CZ2	2.39	0.57
1:A:296:THR:HG23	1:A:299:ALA:H	1.69	0.57
1:A:411:ILE:HG21	1:A:414:TRP:CD1	2.39	0.57
1:B:356:ARG:HH12	1:B:358:ARG:NH2	1.98	0.57
1:B:50:ILE:HG23	1:B:145:GLN:HB3	1.85	0.57
1:A:358:ARG:O	1:A:358:ARG:HD3	2.05	0.57
1:B:266:TRP:CZ3	1:B:427:TYR:CZ	2.93	0.57
1:B:363:ASN:HB3	1:B:366:LYS:HB2	1.86	0.57
1:B:323:LYS:NZ	3:B:2068:HOH:O	2.36	0.57
1:A:92:LEU:HD12	1:A:92:LEU:C	2.28	0.57
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.16	0.57
1:B:274:ILE:O	1:B:275:LYS:HE2	2.04	0.57
1:A:479:LEU:HD11	1:A:501:TYR:HE2	1.69	0.57
1:A:284:ARG:O	1:A:284:ARG:HG3	2.05	0.57
1:B:68:SER:O	1:B:68:SER:OG	2.21	0.57
1:A:379:SER:HB3	1:A:383:TRP:HE3	1.69	0.56
1:B:156:SER:HB2	1:B:157:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:O	1:A:91:GLN:N	2.38	0.56
1:A:460:ASN:HD22	1:B:288:ALA:HB2	1.70	0.56
1:B:63:ILE:HD12	1:B:407:GLN:HA	1.86	0.56
1:B:276:VAL:O	1:B:276:VAL:HG22	2.05	0.56
1:B:331:LYS:O	1:B:424:LYS:HD2	2.04	0.56
1:A:92:LEU:HD12	1:A:92:LEU:O	2.04	0.56
1:A:195:ILE:HG22	1:A:199:ARG:CD	2.34	0.56
1:A:357:MET:HE2	1:A:360:ALA:HB3	1.88	0.56
1:A:518:VAL:O	1:A:522:ILE:HD12	2.05	0.56
1:B:156:SER:HB2	1:B:157:PRO:CD	2.36	0.56
1:B:246:LEU:HB3	1:B:260:LEU:HD11	1.88	0.56
1:B:295:LEU:HD22	1:B:300:GLU:OE2	2.05	0.56
1:A:20:LYS:HE2	1:A:56:TYR:CE1	2.40	0.56
1:A:52:PRO:HD2	1:A:53:GLU:CG	2.26	0.56
1:A:206:ARG:HH21	1:A:218:ASP:CA	2.19	0.56
1:A:164:MET:CE	1:A:187:LEU:HD22	2.36	0.56
1:A:320:ASP:OD1	1:A:322:SER:OG	2.24	0.56
1:A:335:GLY:HA2	1:A:367:GLN:CD	2.31	0.56
1:A:228:LEU:N	1:A:228:LEU:HD23	2.19	0.56
1:A:398:TRP:CZ2	1:A:409:THR:HG23	2.40	0.56
1:A:40:GLU:OE2	1:A:43:LYS:HD3	2.06	0.56
1:A:420:PRO:HA	1:A:421:PRO:C	2.31	0.56
1:A:433:PRO:CG	1:B:255:ASN:ND2	2.68	0.56
1:A:228:LEU:CB	1:A:242:GLN:HE22	2.18	0.56
1:A:258:GLN:CG	1:A:283:LEU:HD22	2.36	0.56
1:B:243:PRO:HA	1:B:310:LEU:O	2.06	0.56
1:B:363:ASN:CG	1:B:366:LYS:HB2	2.30	0.56
1:A:486:LEU:HD13	1:A:524:GLN:HB3	1.89	0.55
1:B:420:PRO:HB2	1:B:423:VAL:HG23	1.88	0.55
1:B:41:MET:CE	1:B:47:ILE:HG23	2.36	0.55
1:B:125:ARG:O	1:B:145:GLN:HG3	2.06	0.55
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.24	0.55
1:A:275:LYS:HG2	1:A:332:GLN:HE22	1.71	0.55
1:A:434:ILE:HB	1:A:437:ALA:HB3	1.89	0.55
1:B:298:GLU:HA	1:B:301:LEU:HD22	1.89	0.55
1:A:210:LEU:C	1:A:212:TRP:N	2.63	0.55
1:B:27:THR:O	1:B:31:ILE:HG13	2.07	0.55
1:B:356:ARG:HH12	1:B:358:ARG:HH21	1.53	0.55
1:A:61:PHE:CE2	1:A:63:ILE:HD12	2.42	0.55
1:A:228:LEU:CA	1:A:242:GLN:HE22	2.20	0.55
1:B:155:GLY:O	1:B:158:ALA:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TRP:H	1:A:24:TRP:CD1	2.23	0.55
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.89	0.55
1:B:81:ASN:OD1	1:B:153:TRP:HD1	1.90	0.55
1:A:88:TRP:HB2	1:B:54:ASN:O	2.07	0.55
1:A:358:ARG:HE	1:A:358:ARG:HA	1.72	0.55
1:B:257:ILE:O	1:B:261:VAL:HG23	2.06	0.55
1:B:328:GLU:OE2	1:B:342:TYR:OH	2.25	0.55
1:A:271:TYR:CZ	1:A:314:VAL:HG23	2.42	0.55
1:B:266:TRP:O	1:B:269:GLN:HB2	2.07	0.55
1:B:272:PRO:C	1:B:274:ILE:H	2.15	0.55
1:A:5:ILE:CD1	1:A:167:ILE:HG13	2.32	0.54
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.43	0.54
1:A:191:SER:OG	1:A:193:LEU:HB2	2.08	0.54
1:B:46:LYS:HD3	1:B:116:PHE:HB3	1.89	0.54
1:A:193:LEU:O	1:A:194:GLU:HB3	2.06	0.54
1:A:295:LEU:HD13	3:A:2099:HOH:O	2.06	0.54
1:B:292:VAL:HG12	1:B:293:ILE:N	2.22	0.54
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.23	0.54
1:A:27:THR:O	1:A:31:ILE:HG13	2.07	0.54
1:A:113:ASP:O	1:A:117:SER:OG	2.25	0.54
1:A:351:THR:HG23	1:A:352:GLY:H	1.71	0.54
1:B:216:THR:H	1:B:217:PRO:HD3	1.73	0.54
1:B:282:LEU:HD12	1:B:282:LEU:H	1.73	0.54
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.43	0.54
1:A:376:THR:HG23	1:A:386:THR:HG22	1.88	0.54
1:B:169:GLU:O	1:B:173:LYS:HB2	2.08	0.54
1:B:425:LEU:O	1:B:425:LEU:HD22	2.08	0.54
1:A:205:LEU:O	1:A:208:HIS:HB3	2.08	0.54
1:A:402:TRP:CZ3	1:B:364:ASP:HB2	2.43	0.54
1:A:426:TRP:O	1:A:526:ILE:HG23	2.08	0.54
1:A:513:SER:CB	1:A:518:VAL:HG11	2.37	0.54
1:A:521:ILE:HG22	1:A:525:LEU:HD12	1.89	0.54
1:B:122:GLU:HB3	3:B:2038:HOH:O	2.08	0.54
1:A:480:GLN:O	1:A:483:TYR:HB3	2.08	0.54
1:B:175:ASN:CB	1:B:178:ILE:HG13	2.38	0.54
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.37	0.54
1:A:471:ASP:HB3	3:A:2135:HOH:O	2.08	0.54
1:A:312:GLU:OE2	1:A:312:GLU:O	2.27	0.53
1:A:502:ALA:O	1:A:506:ILE:HG13	2.09	0.53
1:B:70:LYS:O	1:B:70:LYS:HG3	2.09	0.53
1:B:104:LYS:HD2	1:B:192:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:HG21	1:B:429:LEU:CD2	2.38	0.53
1:A:194:GLU:C	1:A:196:GLY:H	2.17	0.53
1:A:253:THR:HG23	1:A:256:ASP:OD1	2.08	0.53
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.38	0.53
1:A:402:TRP:CD1	1:A:403:THR:CG2	2.88	0.53
1:B:12:LEU:HD12	1:B:127:TYR:CZ	2.43	0.53
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.43	0.53
1:A:65:LYS:N	3:A:2026:HOH:O	2.40	0.53
1:A:194:GLU:C	1:A:196:GLY:N	2.67	0.53
1:A:206:ARG:O	1:A:208:HIS:N	2.41	0.53
1:A:216:THR:CG2	1:A:217:PRO:N	2.72	0.53
1:A:419:THR:O	1:A:419:THR:CG2	2.55	0.53
1:B:72:ARG:NH2	1:B:151:GLN:NE2	2.56	0.53
1:A:156:SER:N	1:A:157:PRO:CD	2.71	0.53
1:A:223:LYS:HG2	3:A:2041:HOH:O	2.08	0.53
1:A:254:VAL:HG23	1:A:291:GLU:HB3	1.91	0.53
1:B:161:GLN:O	1:B:165:THR:HG22	2.08	0.53
1:B:246:LEU:HD12	1:B:307:ARG:HG2	1.91	0.53
1:B:260:LEU:HD23	1:B:279:LEU:HD13	1.91	0.53
1:A:406:TRP:HZ3	1:B:418:ASN:CA	2.20	0.52
1:B:266:TRP:CH2	1:B:427:TYR:CE2	2.97	0.52
1:A:169:GLU:O	1:A:171:PHE:N	2.42	0.52
1:A:308:GLU:O	1:A:311:LYS:HB2	2.09	0.52
1:A:27:THR:HB	1:A:30:LYS:CD	2.40	0.52
1:A:238:LYS:HE3	1:A:315:HIS:ND1	2.24	0.52
1:A:14:PRO:C	1:A:16:MET:H	2.17	0.52
1:B:33:ALA:O	1:B:37:ILE:HD12	2.08	0.52
1:A:20:LYS:HZ1	1:A:55:PRO:HB2	1.73	0.52
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.89	0.52
1:A:351:THR:HG23	1:A:352:GLY:N	2.24	0.52
1:A:489:SER:HB2	1:A:493:VAL:HB	1.90	0.52
1:A:538:ALA:CB	1:A:545:ASN:HD21	2.22	0.52
1:B:13:LYS:HG3	1:B:83:ARG:O	2.09	0.52
1:A:255:ASN:O	1:A:258:GLN:N	2.40	0.52
1:A:351:THR:CG2	1:A:352:GLY:N	2.72	0.52
1:B:66:LYS:HB2	1:B:407:GLN:HB3	1.91	0.52
1:A:451:LYS:NZ	1:A:451:LYS:CB	2.70	0.52
1:A:536:VAL:HG23	1:A:536:VAL:O	2.09	0.52
1:B:278:GLN:O	1:B:281:LYS:HB2	2.09	0.52
1:A:94:ILE:CD1	1:A:95:PRO:HD2	2.30	0.52
1:B:118:VAL:HG11	1:B:149:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LYS:HG2	1:B:417:VAL:HG11	1.92	0.52
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.46	0.51
1:A:265:ASN:C	1:A:268:SER:HB3	2.35	0.51
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.46	0.51
1:B:101:LYS:HG2	3:B:2081:HOH:O	2.10	0.51
1:B:421:PRO:HD2	1:B:422:LEU:H	1.75	0.51
1:A:56:TYR:O	1:A:57:ASN:HB2	2.10	0.51
1:A:115:TYR:HB3	1:A:149:LEU:HB2	1.92	0.51
1:A:208:HIS:O	1:A:212:TRP:HD1	1.93	0.51
1:B:91:GLN:HB3	1:B:92:LEU:HD23	1.92	0.51
1:B:148:VAL:O	1:B:149:LEU:C	2.54	0.51
1:B:379:SER:OG	1:B:387:PRO:HD3	2.09	0.51
1:A:224:GLU:HB2	1:A:225:PRO:CD	2.36	0.51
1:B:193:LEU:HB3	1:B:197:GLN:HB3	1.92	0.51
1:A:493:VAL:HG22	1:A:494:ASN:O	2.11	0.51
1:A:523:GLU:O	1:A:524:GLN:O	2.29	0.51
1:B:314:VAL:HG11	1:B:317:VAL:HG11	1.93	0.51
1:A:71:TRP:CD1	1:A:71:TRP:N	2.79	0.51
1:A:111:VAL:HG11	1:A:214:LEU:HD22	1.91	0.51
1:A:253:THR:OG1	1:A:289:LEU:O	2.24	0.51
1:B:97:PRO:HG3	1:B:181:TYR:HB2	1.92	0.51
1:A:134:SER:O	1:A:137:ASN:N	2.39	0.51
1:A:188:TYR:OH	1:A:229:TRP:NE1	2.42	0.51
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.32	0.51
1:A:521:ILE:HG22	1:A:525:LEU:CD1	2.40	0.51
1:A:521:ILE:O	1:A:525:LEU:HD12	2.10	0.51
1:A:63:ILE:O	1:A:71:TRP:HB3	2.11	0.51
1:A:93:GLY:C	1:B:137:ASN:ND2	2.68	0.51
1:A:230:MET:HE3	3:A:2079:HOH:O	2.11	0.51
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.93	0.51
1:A:402:TRP:HE3	1:A:409:THR:HG22	1.74	0.51
1:B:85:GLN:HA	1:B:88:TRP:CE2	2.46	0.51
1:B:150:PRO:HG2	1:B:153:TRP:HB3	1.92	0.51
1:B:22:LYS:O	1:B:59:PRO:HG3	2.11	0.51
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.51
1:A:406:TRP:CD1	1:A:406:TRP:N	2.75	0.51
1:B:72:ARG:HH21	1:B:151:GLN:HE22	1.59	0.51
1:B:312:GLU:OE1	1:B:312:GLU:HA	2.11	0.51
1:A:228:LEU:N	1:A:228:LEU:CD2	2.74	0.50
1:A:434:ILE:HB	1:A:437:ALA:CB	2.42	0.50
1:A:503:LEU:HD11	1:A:507:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASN:HD21	1:B:201:LYS:CE	2.17	0.50
1:B:319:TYR:CD1	1:B:383:TRP:CD1	2.99	0.50
1:A:129:ALA:HA	1:A:144:TYR:O	2.11	0.50
1:A:171:PHE:CE2	1:A:205:LEU:HA	2.46	0.50
1:B:13:LYS:HB2	1:B:16:MET:CE	2.30	0.50
1:A:183:TYR:OH	1:A:184:MET:HE2	2.11	0.50
1:A:270:ILE:HG23	1:A:271:TYR:HD2	1.76	0.50
1:A:361:HIS:ND1	1:A:505:ILE:HD13	2.26	0.50
1:B:38:CYS:SG	1:B:132:ILE:HD11	2.50	0.50
1:B:332:GLN:HB2	1:B:336:GLN:HB2	1.93	0.50
1:A:157:PRO:HD2	3:A:2053:HOH:O	2.11	0.50
1:A:11:LYS:O	1:A:85:GLN:HG2	2.12	0.50
1:A:405:TYR:CE1	1:A:406:TRP:NE1	2.79	0.50
1:B:247:PRO:C	1:B:307:ARG:HH12	2.20	0.50
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.47	0.50
1:A:153:TRP:CD1	1:A:154:LYS:H	2.30	0.50
1:A:209:LEU:O	1:A:212:TRP:HB2	2.12	0.50
1:A:341:ILE:N	1:A:350:LYS:O	2.35	0.50
1:A:20:LYS:HE2	1:A:56:TYR:CD1	2.47	0.50
1:A:451:LYS:HB3	1:A:451:LYS:HZ3	1.73	0.50
1:A:494:ASN:N	1:A:494:ASN:ND2	2.60	0.50
1:A:138:GLU:HG2	3:A:2048:HOH:O	2.10	0.50
1:A:398:TRP:CH2	1:A:409:THR:CG2	2.95	0.50
1:A:240:THR:HG23	1:A:241:VAL:O	2.12	0.50
1:A:257:ILE:HG22	1:A:283:LEU:CD1	2.33	0.50
1:B:360:ALA:CB	1:B:366:LYS:NZ	2.75	0.50
1:A:228:LEU:CB	1:A:242:GLN:NE2	2.75	0.49
1:A:357:MET:C	1:A:359:GLY:N	2.68	0.49
1:A:469:LEU:HD13	1:A:477:THR:HG22	1.93	0.49
1:A:393:ILE:O	1:A:416:PHE:HD1	1.95	0.49
1:B:209:LEU:CD2	1:B:214:LEU:HD12	2.31	0.49
1:A:136:ASN:H	1:A:138:GLU:HG3	1.77	0.49
1:A:238:LYS:HE3	1:A:315:HIS:CE1	2.48	0.49
1:A:271:TYR:CE1	1:A:314:VAL:CG2	2.95	0.49
1:A:328:GLU:OE2	1:A:342:TYR:OH	2.24	0.49
1:A:498:ASP:CB	1:A:538:ALA:HB2	2.42	0.49
1:A:334:GLN:NE2	1:A:334:GLN:N	2.60	0.49
1:B:168:LEU:HD13	1:B:180:ILE:HG21	1.94	0.49
1:A:396:GLU:HA	1:A:399:GLU:HG2	1.95	0.49
1:A:503:LEU:HD11	1:A:507:GLN:HE22	1.77	0.49
1:B:12:LEU:CD1	1:B:127:TYR:CZ	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:TYR:O	1:B:351:THR:HA	2.12	0.49
1:A:296:THR:HG23	1:A:298:GLU:N	2.27	0.49
1:B:212:TRP:CD1	1:B:212:TRP:N	2.77	0.49
1:A:41:MET:SD	1:A:73:LYS:NZ	2.86	0.49
1:A:265:ASN:CA	1:A:268:SER:HB3	2.43	0.49
1:B:178:ILE:HD11	1:B:201:LYS:HG2	1.95	0.49
1:A:1:PRO:O	1:A:2:ILE:CG1	2.61	0.49
1:A:249:LYS:NZ	1:A:249:LYS:CB	2.75	0.49
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.12	0.49
1:B:245:VAL:HG21	1:B:429:LEU:HD22	1.95	0.49
1:B:247:PRO:O	1:B:307:ARG:NH2	2.46	0.49
1:B:266:TRP:CH2	1:B:427:TYR:OH	2.63	0.49
1:A:241:VAL:HG11	1:A:267:ALA:HA	1.94	0.49
1:A:391:LEU:HD23	1:A:391:LEU:N	2.27	0.49
1:A:391:LEU:C	1:A:393:ILE:H	2.20	0.49
1:A:296:THR:HG22	1:A:299:ALA:CB	2.43	0.49
1:B:93:GLY:O	1:B:95:PRO:HD3	2.13	0.49
1:B:28:GLU:HB2	1:B:135:ILE:CD1	2.33	0.48
1:B:116:PHE:HD2	3:B:2034:HOH:O	1.94	0.48
1:A:27:THR:HG22	1:A:30:LYS:H	1.78	0.48
1:A:79:GLU:CG	1:A:83:ARG:HH11	2.26	0.48
1:A:246:LEU:HD21	1:A:310:LEU:HD13	1.95	0.48
1:A:308:GLU:HA	1:A:311:LYS:HD2	1.95	0.48
1:A:358:ARG:HA	1:A:358:ARG:NE	2.28	0.48
1:A:360:ALA:O	1:A:361:HIS:HB2	2.13	0.48
1:A:434:ILE:CG1	1:A:494:ASN:HD21	2.22	0.48
1:B:360:ALA:HB2	1:B:366:LYS:NZ	2.28	0.48
1:A:486:LEU:HD13	1:A:524:GLN:CB	2.43	0.48
1:B:44:GLU:HB2	1:B:46:LYS:HG3	1.95	0.48
1:A:529:GLU:O	1:A:529:GLU:HG3	2.12	0.48
1:B:22:LYS:HD3	3:B:2007:HOH:O	2.14	0.48
1:B:210:LEU:HD12	1:B:210:LEU:C	2.31	0.48
1:B:41:MET:HE2	1:B:47:ILE:HG23	1.94	0.48
1:B:111:VAL:HG23	1:B:111:VAL:O	2.13	0.48
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.77	0.48
1:B:242:GLN:OE1	1:B:242:GLN:O	2.31	0.48
1:B:402:TRP:O	1:B:406:TRP:HB2	2.14	0.48
1:A:52:PRO:HD2	1:A:53:GLU:H	1.79	0.48
1:A:168:LEU:HD11	1:A:187:LEU:HD21	1.95	0.48
1:A:175:ASN:HD21	1:A:201:LYS:HE3	1.79	0.48
1:B:103:LYS:HG2	1:B:190:GLY:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.29	0.48
1:A:357:MET:C	1:A:359:GLY:H	2.21	0.48
1:A:398:TRP:CE2	1:A:411:ILE:CD1	2.96	0.48
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.49	0.48
1:A:195:ILE:HB	1:A:199:ARG:HD3	1.95	0.48
1:B:317:VAL:HG21	1:B:348:ASN:O	2.14	0.48
1:A:402:TRP:CD1	1:A:403:THR:N	2.82	0.48
1:B:118:VAL:HG12	1:B:149:LEU:CG	2.38	0.48
1:A:101:LYS:HE2	1:A:103:LYS:NZ	2.29	0.47
1:A:270:ILE:HA	1:A:351:THR:HB	1.96	0.47
3:A:2140:HOH:O	1:B:422:LEU:HB2	2.14	0.47
1:B:209:LEU:HD22	1:B:214:LEU:CD1	2.32	0.47
1:B:361:HIS:HB2	3:B:2076:HOH:O	2.14	0.47
1:A:228:LEU:CD1	1:A:242:GLN:NE2	2.75	0.47
1:A:406:TRP:CZ3	1:A:407:GLN:CD	2.93	0.47
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.95	0.47
1:A:490:GLY:O	1:A:492:GLU:N	2.47	0.47
1:B:18:GLY:HA3	1:B:127:TYR:CD1	2.50	0.47
1:B:314:VAL:HG11	1:B:317:VAL:CG1	2.44	0.47
1:A:181:TYR:CD1	1:B:138:GLU:HB3	2.49	0.47
1:A:183:TYR:O	1:A:186:ASP:HB2	2.14	0.47
1:A:448:ARG:H	1:A:448:ARG:HG2	1.55	0.47
1:B:7:THR:O	1:B:9:PRO:HD3	2.14	0.47
1:A:4:PRO:HG2	1:A:212:TRP:CE3	2.50	0.47
1:A:23:GLN:HE22	1:A:60:VAL:N	2.10	0.47
1:A:79:GLU:O	1:A:82:LYS:N	2.47	0.47
1:A:209:LEU:O	1:A:212:TRP:N	2.46	0.47
1:A:276:VAL:O	1:A:276:VAL:HG13	2.14	0.47
1:A:339:TYR:OH	1:A:378:GLU:OE1	2.30	0.47
1:B:154:LYS:HE3	1:B:184:MET:HE2	1.96	0.47
1:B:30:LYS:O	1:B:34:LEU:HG	2.14	0.47
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.49	0.47
1:A:206:ARG:NH2	1:A:218:ASP:CA	2.76	0.47
1:A:224:GLU:CB	1:A:225:PRO:CD	2.92	0.47
1:B:299:ALA:O	1:B:303:LEU:HB2	2.15	0.47
1:B:366:LYS:O	1:B:370:GLU:CG	2.63	0.47
1:A:195:ILE:HB	1:A:199:ARG:CD	2.45	0.47
1:A:218:ASP:HB2	1:A:221:HIS:HD2	1.80	0.47
1:A:365:VAL:HG11	1:A:401:TRP:CE3	2.50	0.47
1:B:120:LEU:O	1:B:125:ARG:NH2	2.36	0.47
1:A:460:ASN:CB	1:B:286:THR:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:THR:HG21	1:B:153:TRP:CE2	2.48	0.47
1:B:363:ASN:CB	1:B:366:LYS:HB2	2.44	0.47
1:A:88:TRP:O	1:A:90:VAL:N	2.46	0.47
1:A:89:GLU:O	1:A:89:GLU:OE1	2.33	0.47
1:A:175:ASN:H	1:A:176:PRO:CD	2.28	0.47
1:A:350:LYS:CG	1:A:351:THR:N	2.78	0.47
1:B:278:GLN:HG3	1:B:299:ALA:N	2.30	0.47
1:B:360:ALA:HB1	3:B:2078:HOH:O	2.14	0.47
1:A:2:ILE:O	1:A:3:SER:C	2.57	0.46
1:A:461:ARG:CG	1:A:461:ARG:NH1	2.72	0.46
1:B:323:LYS:O	1:B:385:LYS:NZ	2.47	0.46
1:B:269:GLN:CG	1:B:346:PHE:CE2	2.97	0.46
1:A:26:LEU:HD12	1:A:133:PRO:HD2	1.96	0.46
1:A:100:LEU:HD21	2:A:1546:I15:N1	2.30	0.46
1:A:459:THR:HG23	1:A:463:ARG:HB2	1.98	0.46
1:B:391:LEU:HD12	1:B:414:TRP:HB2	1.97	0.46
1:A:68:SER:C	1:A:70:LYS:H	2.23	0.46
1:A:197:GLN:HE21	1:A:201:LYS:NZ	2.13	0.46
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.43	0.46
1:A:486:LEU:CD2	1:A:528:LYS:HD2	2.38	0.46
1:B:50:ILE:HD12	1:B:54:ASN:ND2	2.30	0.46
1:B:266:TRP:HZ3	1:B:427:TYR:CZ	2.34	0.46
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.80	0.46
1:A:296:THR:CG2	1:A:299:ALA:N	2.77	0.46
1:B:266:TRP:CD2	1:B:426:TRP:CD1	3.04	0.46
1:B:295:LEU:HD22	1:B:300:GLU:OE1	2.16	0.46
1:B:356:ARG:HD2	1:B:358:ARG:HA	1.98	0.46
1:A:167:ILE:CD1	1:A:214:LEU:HD12	2.45	0.46
1:A:249:LYS:HG2	1:A:251:SER:O	2.16	0.46
1:A:317:VAL:HG13	1:A:318:TYR:N	2.30	0.46
1:A:406:TRP:CZ3	1:B:418:ASN:HA	2.45	0.46
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.62	0.46
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.97	0.46
1:A:27:THR:HG22	1:A:30:LYS:HG2	1.97	0.46
1:A:201:LYS:O	1:A:204:GLU:HB3	2.16	0.46
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.16	0.46
1:A:430:GLU:CD	1:A:530:LYS:HD2	2.41	0.46
1:B:35:VAL:CG1	1:B:36:GLU:N	2.78	0.46
1:A:125:ARG:CG	1:A:146:TYR:O	2.58	0.46
1:A:521:ILE:CG2	1:A:525:LEU:HD11	2.46	0.46
1:B:359:GLY:C	1:B:361:HIS:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.51	0.46
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.16	0.45
1:A:396:GLU:CD	1:A:396:GLU:N	2.65	0.45
1:A:23:GLN:HG2	1:A:57:ASN:HD21	1.81	0.45
1:A:136:ASN:C	1:A:138:GLU:N	2.72	0.45
1:A:173:LYS:HB3	1:A:173:LYS:HE2	1.20	0.45
1:A:180:ILE:HG22	1:A:187:LEU:CD1	2.46	0.45
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.51	0.45
1:A:337:TRP:NE1	1:A:367:GLN:NE2	2.58	0.45
1:A:411:ILE:CG2	1:A:414:TRP:CD1	2.98	0.45
1:A:434:ILE:HG21	1:A:492:GLU:HB3	1.97	0.45
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.49	0.45
1:B:195:ILE:O	1:B:199:ARG:HG2	2.16	0.45
1:B:242:GLN:HB2	1:B:429:LEU:HD11	1.98	0.45
1:A:4:PRO:HD2	1:A:212:TRP:C	2.40	0.45
1:A:135:ILE:HB	1:A:138:GLU:OE2	2.15	0.45
1:A:277:ARG:HG2	1:A:277:ARG:NH1	2.31	0.45
1:A:317:VAL:CG1	1:A:318:TYR:N	2.79	0.45
1:A:335:GLY:HA3	1:A:356:ARG:CD	2.45	0.45
1:A:379:SER:HA	1:A:383:TRP:CE3	2.52	0.45
1:A:440:PHE:CD1	1:A:493:VAL:CG2	2.99	0.45
1:A:447:ASN:O	1:A:451:LYS:N	2.46	0.45
1:A:479:LEU:CD1	1:A:501:TYR:HE2	2.29	0.45
1:B:47:ILE:HB	1:B:145:GLN:O	2.17	0.45
1:A:41:MET:HE1	1:A:73:LYS:HZ3	1.82	0.45
1:B:5:ILE:HD12	1:B:6:GLU:OE1	2.17	0.45
1:B:58:THR:CG2	1:B:75:VAL:HG12	2.46	0.45
1:B:249:LYS:HA	1:B:252:TRP:CE2	2.51	0.45
1:B:295:LEU:HB2	1:B:300:GLU:OE2	2.17	0.45
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.52	0.45
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.84	0.45
1:A:288:ALA:HB3	1:A:291:GLU:OE1	2.17	0.45
1:B:51:GLY:C	1:B:53:GLU:N	2.74	0.45
1:B:245:VAL:CG2	1:B:429:LEU:CD2	2.94	0.45
1:B:266:TRP:HZ3	1:B:427:TYR:HH	1.55	0.45
1:B:312:GLU:HA	1:B:313:PRO:HD2	1.11	0.45
1:A:71:TRP:H	1:A:71:TRP:HD1	1.64	0.45
1:A:244:ILE:HG12	3:A:2083:HOH:O	2.16	0.45
1:B:46:LYS:O	1:B:148:VAL:HG22	2.17	0.45
1:B:292:VAL:CG1	1:B:293:ILE:N	2.79	0.45
1:A:52:PRO:CD	1:A:53:GLU:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PRO:HA	1:A:234:LEU:O	2.17	0.45
1:B:35:VAL:HG12	1:B:36:GLU:N	2.32	0.45
1:B:216:THR:N	1:B:217:PRO:CD	2.78	0.45
1:A:52:PRO:CD	1:A:53:GLU:HG2	2.28	0.45
1:A:167:ILE:HD13	1:A:214:LEU:HD12	1.98	0.45
1:A:529:GLU:O	1:A:530:LYS:HG2	2.16	0.45
1:A:105:SER:CB	1:A:198:HIS:CD2	2.98	0.45
1:A:207:GLN:HG3	3:A:2068:HOH:O	2.17	0.45
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.76	0.44
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.44	0.44
1:A:406:TRP:CZ3	1:A:407:GLN:NE2	2.86	0.44
1:B:92:LEU:N	1:B:92:LEU:CD2	2.79	0.44
1:B:249:LYS:O	1:B:250:ASP:HB2	2.16	0.44
1:A:63:ILE:HG12	1:A:65:LYS:NZ	2.33	0.44
1:A:401:TRP:CD1	1:A:425:LEU:HD11	2.53	0.44
1:A:441:TYR:CG	1:A:544:GLY:HA3	2.52	0.44
1:A:169:GLU:HG2	1:A:170:PRO:N	2.33	0.44
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.49	0.44
1:A:364:ASP:HB2	1:A:423:VAL:HG13	1.99	0.44
1:A:513:SER:CB	1:A:518:VAL:CG1	2.96	0.44
1:B:20:LYS:CE	1:B:55:PRO:HB2	2.45	0.44
1:B:58:THR:CG2	1:B:75:VAL:CG1	2.96	0.44
1:B:298:GLU:H	1:B:298:GLU:HG3	1.48	0.44
1:B:354:TYR:CD2	1:B:354:TYR:C	2.96	0.44
1:A:206:ARG:HH11	1:A:206:ARG:CG	2.31	0.44
1:A:210:LEU:O	1:A:212:TRP:N	2.51	0.44
1:A:296:THR:HG22	1:A:299:ALA:N	2.33	0.44
1:A:371:ALA:O	1:A:372:VAL:C	2.61	0.44
1:A:391:LEU:HA	1:A:392:PRO:HD3	1.78	0.44
1:B:261:VAL:HA	1:B:276:VAL:HG21	1.98	0.44
1:B:410:TRP:C	1:B:410:TRP:HE3	2.25	0.44
1:A:201:LYS:HD2	1:A:201:LYS:HA	1.59	0.44
1:A:273:GLY:HA3	1:A:309:ILE:CD1	2.48	0.44
1:B:388:LYS:HE2	1:B:388:LYS:HB3	1.47	0.44
1:A:10:VAL:HG11	1:A:153:TRP:HH2	1.83	0.44
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.68	0.44
1:A:64:LYS:HA	1:A:71:TRP:HB3	2.00	0.44
1:A:136:ASN:HB2	1:A:138:GLU:CG	2.47	0.44
1:A:416:PHE:CE1	1:A:422:LEU:HD13	2.52	0.44
1:B:5:ILE:HD13	1:B:5:ILE:HA	1.69	0.44
1:B:36:GLU:O	1:B:38:CYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LYS:C	1:B:351:THR:CG2	2.91	0.44
1:A:30:LYS:H	1:A:30:LYS:HG2	1.50	0.44
1:A:79:GLU:O	1:A:81:ASN:N	2.51	0.44
1:A:153:TRP:CD1	1:A:154:LYS:N	2.86	0.44
1:A:180:ILE:HG22	1:A:187:LEU:HD11	1.99	0.44
1:A:237:ASP:HB2	3:A:2033:HOH:O	2.18	0.44
1:A:445:ALA:O	1:A:453:GLY:HA3	2.17	0.44
1:B:246:LEU:HB3	1:B:260:LEU:CD1	2.48	0.44
1:A:102:LYS:HB3	1:A:318:TYR:HB2	2.00	0.43
1:A:122:GLU:C	1:A:124:PHE:H	2.26	0.43
1:A:131:THR:OG1	1:A:143:ARG:HG2	2.18	0.43
1:A:450:THR:O	1:A:451:LYS:HB2	2.18	0.43
1:A:521:ILE:CG2	1:A:525:LEU:CD1	2.95	0.43
1:B:78:ARG:O	1:B:82:LYS:HG3	2.18	0.43
1:B:326:ILE:HG12	1:B:388:LYS:CE	2.48	0.43
1:A:27:THR:HB	1:A:30:LYS:CG	2.48	0.43
1:A:136:ASN:HB2	3:A:2048:HOH:O	2.18	0.43
1:A:171:PHE:O	1:A:175:ASN:HB2	2.17	0.43
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.52	0.43
1:A:441:TYR:HB3	1:A:544:GLY:HA3	2.00	0.43
1:A:529:GLU:C	1:A:530:LYS:HG2	2.42	0.43
1:B:94:ILE:N	1:B:94:ILE:CD1	2.73	0.43
1:B:246:LEU:HD12	1:B:307:ARG:CG	2.48	0.43
1:B:341:ILE:HG21	1:B:383:TRP:CZ3	2.52	0.43
1:B:393:ILE:HG12	1:B:394:GLN:H	1.83	0.43
1:A:328:GLU:O	1:A:339:TYR:HA	2.18	0.43
1:A:334:GLN:HB2	3:A:2107:HOH:O	2.18	0.43
1:A:379:SER:HB3	1:A:383:TRP:CE3	2.53	0.43
1:B:13:LYS:CB	1:B:16:MET:CE	2.95	0.43
1:B:118:VAL:HG11	1:B:149:LEU:CD1	2.48	0.43
1:B:214:LEU:N	1:B:214:LEU:CD2	2.79	0.43
1:B:243:PRO:C	1:B:245:VAL:N	2.72	0.43
1:A:467:VAL:HG13	1:A:468:THR:N	2.33	0.43
1:A:511:ASP:OD1	1:A:511:ASP:C	2.62	0.43
1:B:157:PRO:HG3	1:B:184:MET:O	2.18	0.43
1:B:281:LYS:O	1:B:283:LEU:N	2.51	0.43
1:B:376:THR:HG23	1:B:386:THR:HG22	1.99	0.43
1:A:167:ILE:CD1	1:A:214:LEU:CD1	2.96	0.43
1:A:455:ALA:O	1:A:467:VAL:N	2.52	0.43
1:B:391:LEU:O	1:B:393:ILE:N	2.52	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:CG	1:A:298:GLU:CB	2.96	0.43
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.33	0.43
1:A:441:TYR:HB3	1:A:544:GLY:CA	2.49	0.43
1:A:8:VAL:HA	1:A:9:PRO:HD2	1.46	0.43
1:A:277:ARG:NH2	1:A:334:GLN:CG	2.80	0.43
1:A:356:ARG:HB3	1:A:359:GLY:H	1.82	0.43
1:A:448:ARG:CG	1:A:448:ARG:NH1	2.77	0.43
1:A:450:THR:O	1:A:451:LYS:CB	2.67	0.43
1:B:249:LYS:HD3	1:B:250:ASP:H	1.80	0.43
1:B:356:ARG:HH11	1:B:358:ARG:NH2	2.10	0.43
1:B:367:GLN:HA	1:B:370:GLU:HG3	2.01	0.43
1:B:360:ALA:HB3	1:B:366:LYS:HZ3	1.84	0.43
1:A:169:GLU:C	1:A:171:PHE:H	2.27	0.43
1:A:542:ILE:HA	1:B:283:LEU:O	2.19	0.43
1:B:241:VAL:CG2	1:B:242:GLN:N	2.78	0.43
1:B:403:THR:C	1:B:405:TYR:N	2.74	0.43
1:A:254:VAL:HG21	1:A:291:GLU:HB3	1.99	0.43
1:A:273:GLY:HA3	1:A:309:ILE:HD13	2.00	0.43
1:B:132:ILE:O	1:B:133:PRO:O	2.36	0.43
1:B:175:ASN:OD1	1:B:175:ASN:N	2.51	0.43
1:B:274:ILE:CG2	1:B:275:LYS:N	2.82	0.43
1:B:278:GLN:HB2	1:B:302:GLU:CD	2.44	0.43
1:A:102:LYS:HE2	1:A:320:ASP:CB	2.30	0.42
1:A:195:ILE:CB	1:A:199:ARG:CD	2.97	0.42
1:A:376:THR:HG23	1:A:386:THR:CG2	2.49	0.42
1:A:406:TRP:CZ3	1:B:419:THR:N	2.87	0.42
1:A:433:PRO:CG	1:B:255:ASN:HD22	2.31	0.42
1:A:538:ALA:O	1:A:539:HIS:HB2	2.19	0.42
1:B:13:LYS:CE	1:B:16:MET:HE1	2.48	0.42
1:A:183:TYR:CE1	1:A:230:MET:SD	3.12	0.42
1:A:540:LYS:CB	1:A:542:ILE:CD1	2.92	0.42
1:B:51:GLY:HA3	1:B:53:GLU:OE1	2.19	0.42
1:B:346:PHE:HD1	1:B:346:PHE:HA	1.72	0.42
1:B:358:ARG:HB2	3:B:2076:HOH:O	2.19	0.42
1:B:410:TRP:C	1:B:410:TRP:CE3	2.97	0.42
1:A:168:LEU:O	1:A:169:GLU:C	2.61	0.42
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.83	0.42
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.78	0.42
1:B:244:ILE:O	1:B:245:VAL:HG22	2.18	0.42
1:B:350:LYS:HB2	1:B:383:TRP:HH2	1.83	0.42
1:A:246:LEU:HD21	1:A:310:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:O	1:A:258:GLN:HB2	2.19	0.42
1:A:263:LYS:HD3	1:A:263:LYS:HA	1.87	0.42
1:A:328:GLU:OE2	1:A:342:TYR:CE2	2.72	0.42
1:A:356:ARG:HB3	1:A:359:GLY:N	2.34	0.42
1:B:175:ASN:ND2	1:B:201:LYS:CE	2.75	0.42
1:B:243:PRO:HB2	1:B:245:VAL:HG13	2.01	0.42
1:B:421:PRO:CD	1:B:422:LEU:H	2.31	0.42
1:A:3:SER:OG	1:A:5:ILE:HB	2.19	0.42
1:A:153:TRP:CG	1:A:154:LYS:N	2.87	0.42
1:A:169:GLU:C	1:A:171:PHE:N	2.78	0.42
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.50	0.42
1:B:58:THR:HG21	1:B:75:VAL:HG12	2.00	0.42
1:A:3:SER:HA	1:A:4:PRO:HD2	1.81	0.42
1:A:101:LYS:CD	1:A:103:LYS:CE	2.93	0.42
1:A:240:THR:OG1	1:A:241:VAL:N	2.52	0.42
1:A:279:LEU:HG	1:A:302:GLU:OE2	2.20	0.42
1:A:441:TYR:CB	1:A:544:GLY:HA3	2.49	0.42
1:A:379:SER:OG	1:A:387:PRO:HD3	2.19	0.42
1:B:50:ILE:HD11	1:B:129:ALA:HB1	2.02	0.42
1:A:3:SER:HA	1:A:213:GLY:HA3	2.01	0.42
1:A:357:MET:O	1:A:357:MET:HG2	2.20	0.42
1:B:172:ARG:HG3	1:B:172:ARG:NH1	2.35	0.42
1:A:277:ARG:CZ	1:A:334:GLN:CG	2.97	0.42
1:A:334:GLN:O	1:A:336:GLN:HG3	2.20	0.42
1:A:356:ARG:NH1	1:A:512:GLN:NE2	2.66	0.42
1:B:271:TYR:HA	1:B:272:PRO:HD2	1.91	0.42
1:A:203:GLU:CD	1:A:219:LYS:HZ3	2.27	0.42
1:A:268:SER:O	1:A:351:THR:HG22	2.18	0.42
1:A:391:LEU:HB2	1:A:393:ILE:HG22	2.01	0.42
1:A:398:TRP:CZ2	1:A:409:THR:CG2	3.03	0.42
1:B:111:VAL:HG11	1:B:187:LEU:HG	2.02	0.42
1:A:249:LYS:NZ	1:A:249:LYS:HB2	2.18	0.41
1:A:253:THR:OG1	1:A:256:ASP:OD1	2.38	0.41
1:B:266:TRP:HH2	1:B:427:TYR:HH	1.61	0.41
1:B:287:LYS:HD3	1:B:293:ILE:HD11	2.02	0.41
1:B:369:THR:HG22	1:B:398:TRP:CZ3	2.54	0.41
1:B:382:ILE:HG22	1:B:382:ILE:O	2.18	0.41
1:B:425:LEU:HA	1:B:425:LEU:HD23	1.34	0.41
1:A:130:PHE:CD2	1:A:130:PHE:N	2.88	0.41
1:A:202:ILE:HD12	1:A:202:ILE:HA	1.81	0.41
1:A:256:ASP:HA	1:A:259:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:HB3	1:A:274:ILE:CD1	2.50	0.41
1:A:452:LEU:HD23	3:A:2126:HOH:O	2.20	0.41
1:A:501:TYR:O	1:A:505:ILE:HG13	2.20	0.41
1:B:205:LEU:O	1:B:205:LEU:HD12	2.19	0.41
1:B:419:THR:HA	1:B:420:PRO:HD2	1.94	0.41
1:B:34:LEU:HD23	1:B:34:LEU:HA	1.84	0.41
1:B:297:GLU:HA	1:B:300:GLU:HG3	2.01	0.41
1:B:331:LYS:CE	1:B:364:ASP:OD2	2.63	0.41
1:A:107:THR:HG21	1:A:202:ILE:HG21	2.02	0.41
1:A:195:ILE:CG2	1:A:199:ARG:CD	2.98	0.41
1:A:303:LEU:HD12	1:A:303:LEU:C	2.44	0.41
1:A:334:GLN:O	1:A:335:GLY:C	2.62	0.41
1:B:50:ILE:HD12	1:B:54:ASN:CB	2.51	0.41
1:B:86:ASP:HA	1:B:90:VAL:HG23	2.02	0.41
1:B:242:GLN:O	1:B:242:GLN:CG	2.68	0.41
1:B:266:TRP:CH2	1:B:427:TYR:CZ	3.07	0.41
1:B:333:GLY:O	1:B:334:GLN:HB2	2.19	0.41
1:A:334:GLN:O	1:A:336:GLN:N	2.53	0.41
1:B:21:VAL:HG21	1:B:79:GLU:CG	2.50	0.41
1:B:36:GLU:C	1:B:38:CYS:N	2.77	0.41
1:B:180:ILE:HD13	1:B:189:VAL:HG22	2.02	0.41
1:B:270:ILE:HG21	1:B:270:ILE:HD13	1.85	0.41
1:B:320:ASP:CG	1:B:322:SER:HG	2.28	0.41
1:A:136:ASN:HB2	1:A:138:GLU:HG3	2.02	0.41
1:A:257:ILE:CG2	1:A:283:LEU:CD1	2.97	0.41
1:A:393:ILE:O	1:A:416:PHE:CD1	2.73	0.41
1:A:433:PRO:CD	1:B:255:ASN:ND2	2.83	0.41
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.51	0.41
1:B:132:ILE:HA	1:B:133:PRO:HD2	1.65	0.41
1:B:328:GLU:HG2	1:B:390:LYS:HD2	2.03	0.41
1:A:443:ASP:O	1:A:481:ALA:HB2	2.20	0.41
1:A:542:ILE:HB	1:A:545:ASN:HB3	2.02	0.41
1:A:221:HIS:O	1:A:222:GLN:C	2.64	0.41
1:A:284:ARG:O	1:A:285:GLY:O	2.38	0.41
1:A:491:LEU:HD13	3:A:2149:HOH:O	2.21	0.41
1:B:287:LYS:CD	1:B:293:ILE:HD11	2.51	0.41
1:B:363:ASN:HB3	1:B:366:LYS:CB	2.50	0.41
1:A:183:TYR:HE1	1:A:230:MET:SD	2.44	0.41
1:A:196:GLY:C	1:A:198:HIS:H	2.27	0.41
1:A:238:LYS:HD2	3:A:2082:HOH:O	2.21	0.41
1:A:268:SER:O	1:A:351:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:HIS:CD2	1:A:513:SER:OG	2.74	0.41
1:A:440:PHE:HD1	1:A:493:VAL:HG23	1.86	0.41
1:A:448:ARG:CZ	1:A:448:ARG:HB3	2.51	0.41
1:A:450:THR:HB	1:A:452:LEU:CD1	2.51	0.41
1:A:491:LEU:H	1:A:491:LEU:CD2	2.25	0.41
1:A:513:SER:HB3	1:A:518:VAL:HG12	2.03	0.41
1:A:540:LYS:CB	1:A:542:ILE:HD12	2.35	0.41
1:B:119:PRO:HA	1:B:148:VAL:HA	2.02	0.41
1:B:213:GLY:C	1:B:214:LEU:HD23	2.45	0.41
1:B:264:LEU:CD2	1:B:306:ASN:ND2	2.83	0.41
1:B:339:TYR:OH	1:B:378:GLU:OE1	2.39	0.41
1:B:81:ASN:HD22	1:B:154:LYS:HD2	1.82	0.41
1:B:88:TRP:CZ3	1:B:89:GLU:HB2	2.56	0.41
1:B:100:LEU:HD22	1:B:181:TYR:HB3	2.03	0.41
1:A:63:ILE:CG1	1:A:65:LYS:HZ1	2.33	0.40
1:A:340:GLN:HE21	1:A:340:GLN:HB3	1.57	0.40
1:A:409:THR:HG22	1:A:409:THR:O	2.21	0.40
1:A:467:VAL:CG1	1:A:468:THR:N	2.82	0.40
1:B:103:LYS:CD	1:B:190:GLY:HA3	2.50	0.40
1:A:79:GLU:HG3	1:A:83:ARG:HH11	1.85	0.40
1:A:216:THR:CG2	1:A:217:PRO:CD	2.99	0.40
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.37	0.40
1:A:357:MET:HE2	1:A:357:MET:O	2.21	0.40
1:A:405:TYR:O	1:B:331:LYS:HD3	2.20	0.40
1:A:493:VAL:HG22	1:A:494:ASN:N	2.36	0.40
1:B:231:GLY:CA	1:B:232:TYR:C	2.88	0.40
1:B:356:ARG:HD2	1:B:358:ARG:CA	2.52	0.40
1:A:14:PRO:C	1:A:16:MET:N	2.80	0.40
1:A:34:LEU:HD22	1:A:73:LYS:HG3	2.04	0.40
1:A:136:ASN:H	1:A:138:GLU:CG	2.34	0.40
1:A:164:MET:O	1:A:164:MET:HG3	2.20	0.40
1:A:180:ILE:CG2	1:A:187:LEU:CD1	2.99	0.40
1:A:460:ASN:CA	1:B:286:THR:O	2.68	0.40
1:A:545:ASN:ND2	1:A:545:ASN:C	2.80	0.40
1:B:153:TRP:CZ2	1:B:155:GLY:HA3	2.56	0.40
1:B:171:PHE:HB2	1:B:208:HIS:CD2	2.57	0.40
1:B:376:THR:CG2	1:B:386:THR:CG2	2.98	0.40
1:A:79:GLU:O	1:A:80:LEU:C	2.64	0.40
1:A:395:LYS:CD	1:A:414:TRP:CH2	2.96	0.40
1:B:5:ILE:O	1:B:5:ILE:HG22	2.22	0.40
1:B:161:GLN:HE21	1:B:161:GLN:HB2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLN:HB3	1:B:211:ARG:NH1	2.36	0.40
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.56	0.40
1:A:139:THR:CB	1:A:140:PRO:CD	2.96	0.40
1:A:181:TYR:HB2	1:A:188:TYR:HB2	2.04	0.40
1:B:210:LEU:HD12	1:B:210:LEU:HA	1.71	0.40
1:B:332:GLN:NE2	1:B:428:GLN:HA	2.37	0.40
1:B:339:TYR:CD1	1:B:375:ILE:HG12	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	543/566 (96%)	415 (76%)	86 (16%)	42 (8%)	1	2
1	B	412/566 (73%)	338 (82%)	42 (10%)	32 (8%)	1	2
All	All	955/1132 (84%)	753 (79%)	128 (13%)	74 (8%)	1	2

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	14	PRO
1	A	90	VAL
1	A	135	ILE
1	A	139	THR
1	A	169	GLU
1	A	175	ASN
1	A	251	SER
1	A	287	LYS
1	A	356	ARG
1	A	491	LEU

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Mol	Chain	Res	Type
1	A	524	GLN
1	A	525	LEU
1	A	528	LYS
1	A	542	ILE
1	B	4	PRO
1	B	133	PRO
1	B	232	TYR
1	B	249	LYS
1	B	250	ASP
1	B	313	PRO
1	B	315	HIS
1	A	195	ILE
1	A	196	GLY
1	A	206	ARG
1	A	207	GLN
1	A	243	PRO
1	A	255	ASN
1	A	274	ILE
1	A	285	GLY
1	A	361	HIS
1	A	412	PRO
1	B	241	VAL
1	B	272	PRO
1	B	273	GLY
1	B	282	LEU
1	B	310	LEU
1	B	314	VAL
1	B	345	PRO
1	A	80	LEU
1	A	256	ASP
1	A	335	GLY
1	A	345	PRO
1	B	6	GLU
1	B	9	PRO
1	B	160	PHE
1	B	216	THR
1	B	358	ARG
1	A	3	SER
1	A	140	PRO
1	A	268	SER
1	B	69	THR
1	B	71	TRP

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Mol	Chain	Res	Type
1	B	286	THR
1	B	346	PHE
1	B	350	LYS
1	A	5	ILE
1	A	66	LYS
1	A	303	LEU
1	B	65	LYS
1	B	85	GLN
1	B	119	PRO
1	B	245	VAL
1	B	297	GLU
1	A	57	ASN
1	A	89	GLU
1	A	288	ALA
1	A	490	GLY
1	B	149	LEU
1	B	392	PRO
1	A	170	PRO
1	A	466	VAL
1	B	18	GLY
1	A	276	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	487/505 (96%)	331 (68%)	156 (32%)	0	1
1	B	375/505 (74%)	266 (71%)	109 (29%)	0	1
All	All	862/1010 (85%)	597 (69%)	265 (31%)	0	1

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU

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Mol	Chain	Res	Type
1	A	11	LYS
1	A	12	LEU
1	A	14	PRO
1	A	22	LYS
1	A	24	TRP
1	A	27	THR
1	A	30	LYS
1	A	32	LYS
1	A	42	GLU
1	A	43	LYS
1	A	47	ILE
1	A	58	THR
1	A	60	VAL
1	A	63	ILE
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	68	SER
1	A	69	THR
1	A	71	TRP
1	A	72	ARG
1	A	73	LYS
1	A	74	LEU
1	A	78	ARG
1	A	89	GLU
1	A	90	VAL
1	A	92	LEU
1	A	94	ILE
1	A	103	LYS
1	A	105	SER
1	A	106	VAL
1	A	117	SER
1	A	125	ARG
1	A	126	LYS
1	A	134	SER
1	A	138	GLU
1	A	139	THR
1	A	142	ILE
1	A	162	SER
1	A	165	THR
1	A	173	LYS
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	177	ASP
1	A	179	VAL
1	A	184	MET
1	A	187	LEU
1	A	195	ILE
1	A	199	ARG
1	A	200	THR
1	A	201	LYS
1	A	202	ILE
1	A	203	GLU
1	A	205	LEU
1	A	206	ARG
1	A	207	GLN
1	A	215	THR
1	A	221	HIS
1	A	223	LYS
1	A	228	LEU
1	A	230	MET
1	A	238	LYS
1	A	241	VAL
1	A	244	ILE
1	A	245	VAL
1	A	246	LEU
1	A	249	LYS
1	A	250	ASP
1	A	253	THR
1	A	257	ILE
1	A	259	LYS
1	A	268	SER
1	A	274	ILE
1	A	276	VAL
1	A	280	CYS
1	A	281	LYS
1	A	284	ARG
1	A	289	LEU
1	A	290	THR
1	A	292	VAL
1	A	296	THR
1	A	300	GLU
1	A	301	LEU
1	A	305	GLU
1	A	311	LYS

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Mol	Chain	Res	Type
1	A	312	GLU
1	A	313	PRO
1	A	314	VAL
1	A	317	VAL
1	A	326	ILE
1	A	331	LYS
1	A	332	GLN
1	A	334	GLN
1	A	338	THR
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	347	LYS
1	A	350	LYS
1	A	351	THR
1	A	356	ARG
1	A	357	MET
1	A	369	THR
1	A	374	LYS
1	A	378	GLU
1	A	379	SER
1	A	381	VAL
1	A	390	LYS
1	A	391	LEU
1	A	396	GLU
1	A	399	GLU
1	A	400	THR
1	A	402	TRP
1	A	404	GLU
1	A	409	THR
1	A	424	LYS
1	A	428	GLN
1	A	429	LEU
1	A	434	ILE
1	A	439	THR
1	A	448	ARG
1	A	451	LYS
1	A	458	VAL
1	A	459	THR
1	A	461	ARG
1	A	463	ARG
1	A	464	GLN

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Mol	Chain	Res	Type
1	A	465	LYS
1	A	466	VAL
1	A	468	THR
1	A	470	THR
1	A	471	ASP
1	A	478	GLU
1	A	480	GLN
1	A	484	LEU
1	A	488	ASP
1	A	494	ASN
1	A	496	VAL
1	A	498	ASP
1	A	499	SER
1	A	505	ILE
1	A	507	GLN
1	A	512	GLN
1	A	515	SER
1	A	517	LEU
1	A	518	VAL
1	A	520	GLN
1	A	522	ILE
1	A	523	GLU
1	A	524	GLN
1	A	527	LYS
1	A	528	LYS
1	A	529	GLU
1	A	540	LYS
1	A	545	ASN
1	B	5	ILE
1	B	10	VAL
1	B	11	LYS
1	B	16	MET
1	B	22	LYS
1	B	32	LYS
1	B	35	VAL
1	B	40	GLU
1	B	42	GLU
1	B	48	SER
1	B	58	THR
1	B	63	ILE
1	B	65	LYS
1	B	67	ASP

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Mol	Chain	Res	Type
1	B	68	SER
1	B	69	THR
1	B	70	LYS
1	B	73	LYS
1	B	84	THR
1	B	85	GLN
1	B	86	ASP
1	B	90	VAL
1	B	92	LEU
1	B	94	ILE
1	B	101	LYS
1	B	103	LYS
1	B	109	LEU
1	B	113	ASP
1	B	117	SER
1	B	118	VAL
1	B	125	ARG
1	B	134	SER
1	B	138	GLU
1	B	154	LYS
1	B	165	THR
1	B	166	LYS
1	B	169	GLU
1	B	172	ARG
1	B	174	GLN
1	B	175	ASN
1	B	178	ILE
1	B	179	VAL
1	B	180	ILE
1	B	182	GLN
1	B	201	LYS
1	B	203	GLU
1	B	206	ARG
1	B	211	ARG
1	B	214	LEU
1	B	215	THR
1	B	216	THR
1	B	233	GLU
1	B	240	THR
1	B	241	VAL
1	B	242	GLN
1	B	244	ILE

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	249	LYS
1	B	250	ASP
1	B	256	ASP
1	B	264	LEU
1	B	265	ASN
1	B	268	SER
1	B	269	GLN
1	B	274	ILE
1	B	275	LYS
1	B	277	ARG
1	B	278	GLN
1	B	279	LEU
1	B	280	CYS
1	B	282	LEU
1	B	284	ARG
1	B	286	THR
1	B	289	LEU
1	B	290	THR
1	B	291	GLU
1	B	295	LEU
1	B	298	GLU
1	B	301	LEU
1	B	305	GLU
1	B	307	ARG
1	B	308	GLU
1	B	311	LYS
1	B	314	VAL
1	B	317	VAL
1	B	325	LEU
1	B	326	ILE
1	B	329	ILE
1	B	338	THR
1	B	344	GLU
1	B	349	LEU
1	B	350	LYS
1	B	353	LYS
1	B	356	ARG
1	B	358	ARG
1	B	362	THR
1	B	364	ASP
1	B	366	LYS

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Mol	Chain	Res	Type
1	B	369	THR
1	B	370	GLU
1	B	378	GLU
1	B	388	LYS
1	B	392	PRO
1	B	393	ILE
1	B	395	LYS
1	B	413	GLU
1	B	424	LYS
1	B	425	LEU
1	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	96	HIS
1	A	161	GLN
1	A	174	GLN
1	A	182	GLN
1	A	197	GLN
1	A	221	HIS
1	A	222	GLN
1	A	242	GLN
1	A	269	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	367	GLN
1	A	475	GLN
1	A	480	GLN
1	A	494	ASN
1	A	500	GLN
1	A	507	GLN
1	A	512	GLN
1	A	519	ASN
1	A	524	GLN
1	A	545	ASN
1	B	54	ASN
1	B	91	GLN
1	B	137	ASN
1	B	151	GLN

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Mol	Chain	Res	Type
1	B	208	HIS
1	B	255	ASN
1	B	315	HIS
1	B	334	GLN
1	B	336	GLN
1	B	428	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	I15	A	1546	-	23,24,24	2.06	9 (39%)	31,34,34	2.27	13 (41%)

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
2	I15	A	1546	-	-	1/8/8/8	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1546	I15	C1-C4	4.97	1.47	1.43
2	A	1546	I15	C12-C6	3.25	1.44	1.37
2	A	1546	I15	C3-N7	3.19	1.42	1.36
2	A	1546	I15	F1-C6	3.13	1.43	1.35
2	A	1546	I15	C12-C8	2.99	1.43	1.38
2	A	1546	I15	C13-C15	-2.90	1.34	1.39
2	A	1546	I15	C10-C4	-2.36	1.45	1.50
2	A	1546	I15	C14-C11	2.11	1.42	1.39
2	A	1546	I15	C16-C19	-2.01	1.40	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1546	I15	C10-C4-C1	-6.27	123.36	129.96
2	A	1546	I15	C12-C6-C2	-3.69	115.23	122.86
2	A	1546	I15	C3-N7-N9	3.54	114.53	111.90
2	A	1546	I15	C16-C14-C11	-3.41	115.21	119.30
2	A	1546	I15	C3-C1-C2	3.03	120.68	117.70
2	A	1546	I15	C17-C16-C14	2.93	124.24	119.70
2	A	1546	I15	C11-O5-C2	2.60	122.50	118.40
2	A	1546	I15	F1-C6-C12	2.42	124.26	118.65
2	A	1546	I15	C3-C1-C4	2.41	107.37	104.88
2	A	1546	I15	C15-C13-C11	2.29	122.06	119.30
2	A	1546	I15	C8-C3-N7	2.20	138.65	132.62
2	A	1546	I15	C17-C15-C18	2.18	122.50	119.55
2	A	1546	I15	F1-C6-C2	2.17	120.50	117.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

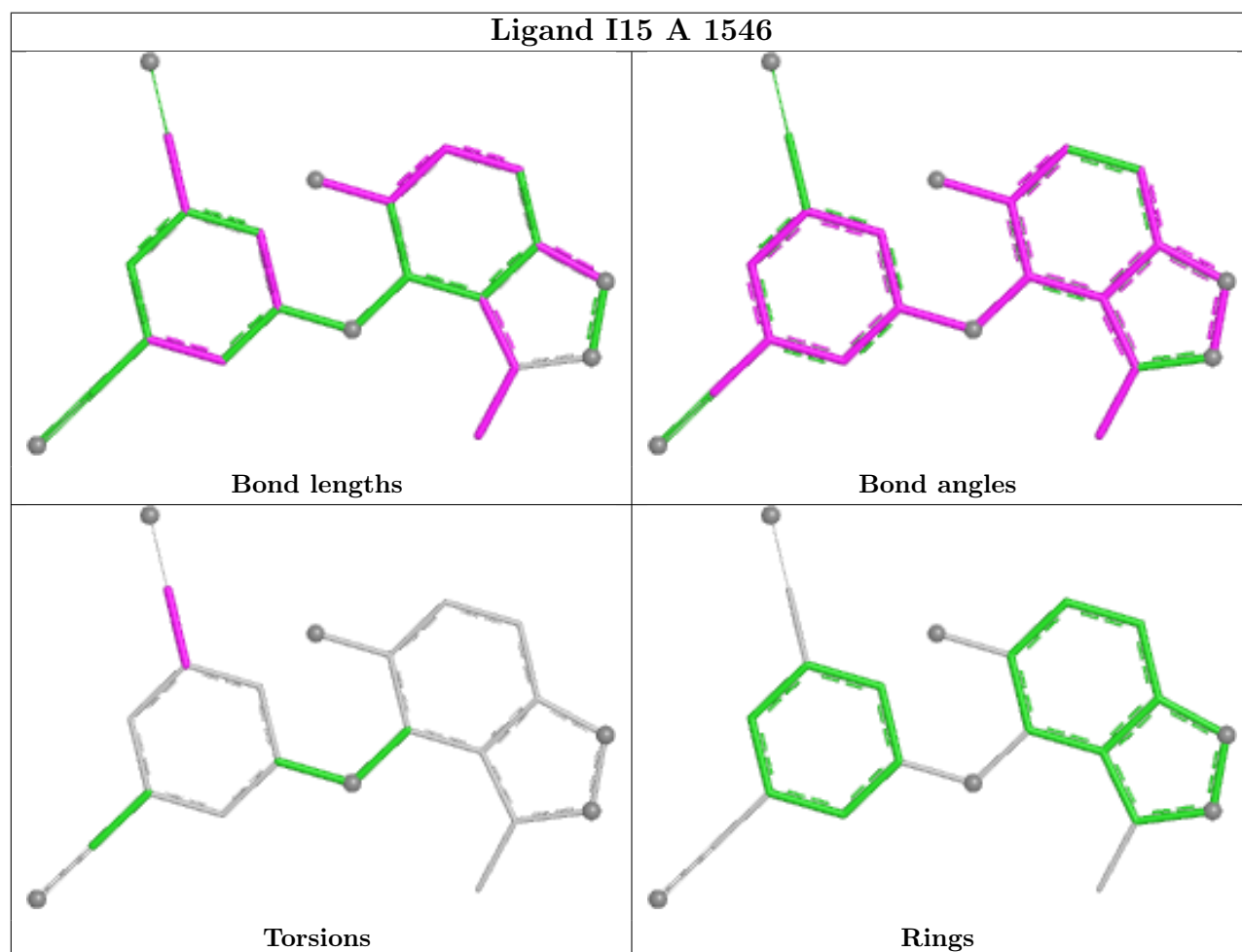
Mol	Chain	Res	Type	Atoms
2	A	1546	I15	C17-C16-C19-N23

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1546	I15	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	545/566 (96%)	0.50	26 (4%)	35 28	34, 59, 86, 107	0
1	B	416/566 (73%)	0.57	25 (6%)	27 21	36, 58, 95, 119	0
All	All	961/1132 (84%)	0.53	51 (5%)	32 25	34, 59, 90, 119	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	GLY	4.8
1	A	402	TRP	4.1
1	B	357	MET	3.9
1	A	24	TRP	3.6
1	A	65	LYS	3.5
1	B	4	PRO	3.2
1	B	5	ILE	3.2
1	A	195	ILE	2.8
1	B	14	PRO	2.8
1	B	278	GLN	2.7
1	A	544	GLY	2.7
1	A	289	LEU	2.7
1	A	290	THR	2.7
1	B	231	GLY	2.7
1	B	362	THR	2.7
1	B	232	TYR	2.6
1	A	542	ILE	2.6
1	B	230	MET	2.6
1	B	360	ALA	2.6
1	A	52	PRO	2.4
1	A	292	VAL	2.4
1	B	430	GLU	2.4
1	B	16	MET	2.4
1	B	244	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	2.4
1	A	291	GLU	2.4
1	A	301	LEU	2.4
1	B	284	ARG	2.3
1	B	301	LEU	2.3
1	B	116	PHE	2.3
1	B	137	ASN	2.2
1	B	421	PRO	2.2
1	A	255	ASN	2.2
1	A	520	GLN	2.2
1	A	315	HIS	2.2
1	A	177	ASP	2.2
1	A	217	PRO	2.2
1	A	251	SER	2.2
1	A	123	ASP	2.1
1	A	396	GLU	2.1
1	A	545	ASN	2.1
1	B	295	LEU	2.1
1	B	169	GLU	2.1
1	B	217	PRO	2.1
1	B	213	GLY	2.1
1	A	288	ALA	2.1
1	A	357	MET	2.1
1	B	65	LYS	2.0
1	B	40	GLU	2.0
1	B	268	SER	2.0
1	A	360	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

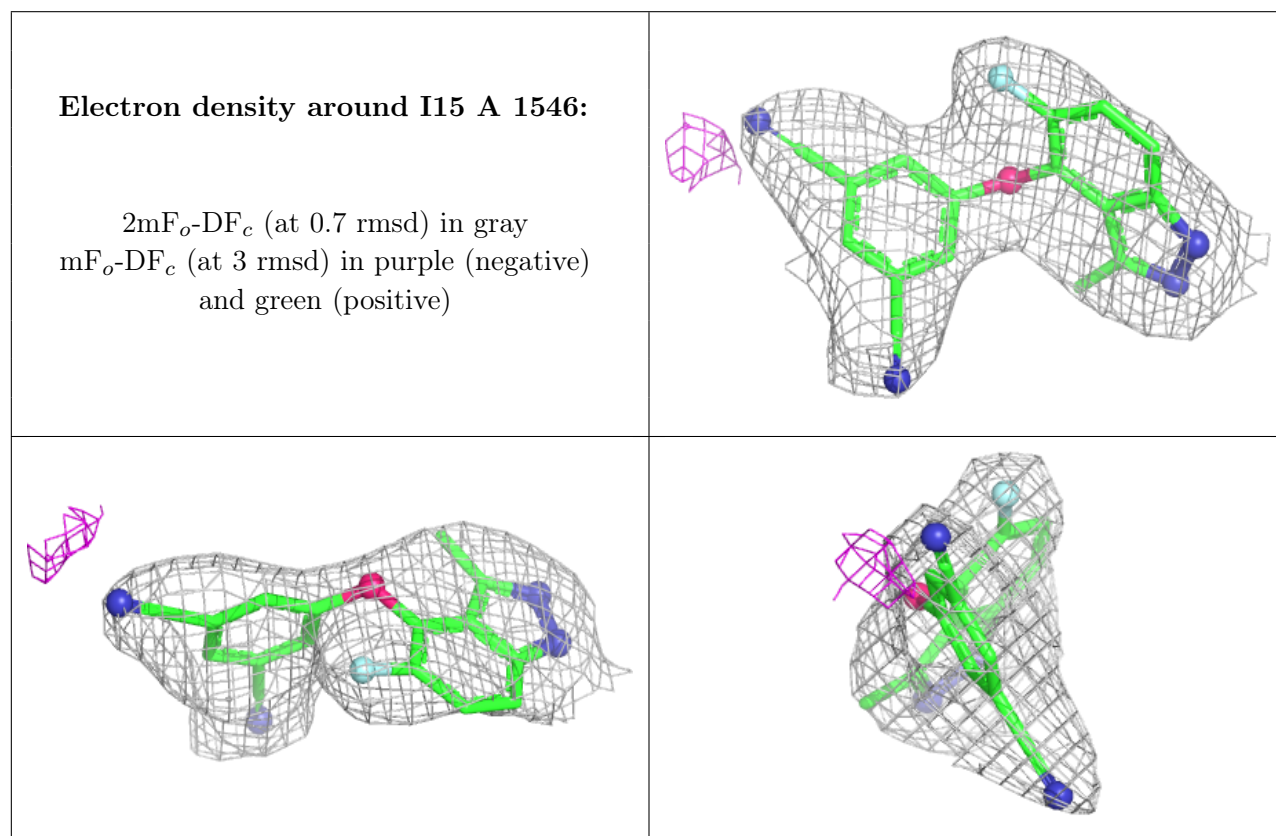
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	I15	A	1546	22/22	0.91	0.10	42,51,55,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.