



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:38 PM UTC

PDB ID : 3G8E / pdb_00003g8e
Title : Crystal Structure of Rattus norvegicus Visfatin/PBEF/Nampt in Complex with an FK866-based inhibitor
Authors : Kang, G.B.; Bae, M.H.; Kim, M.K.; Im, I.; Kim, Y.C.; Eom, S.H.
Deposited on : 2009-02-12
Resolution : 3.00 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

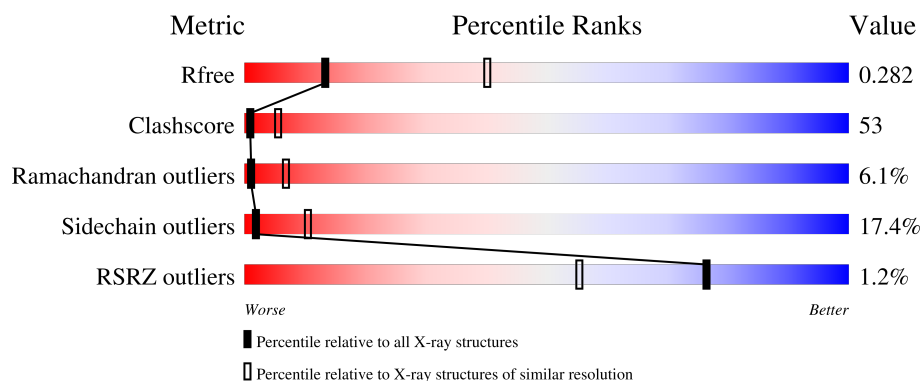
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

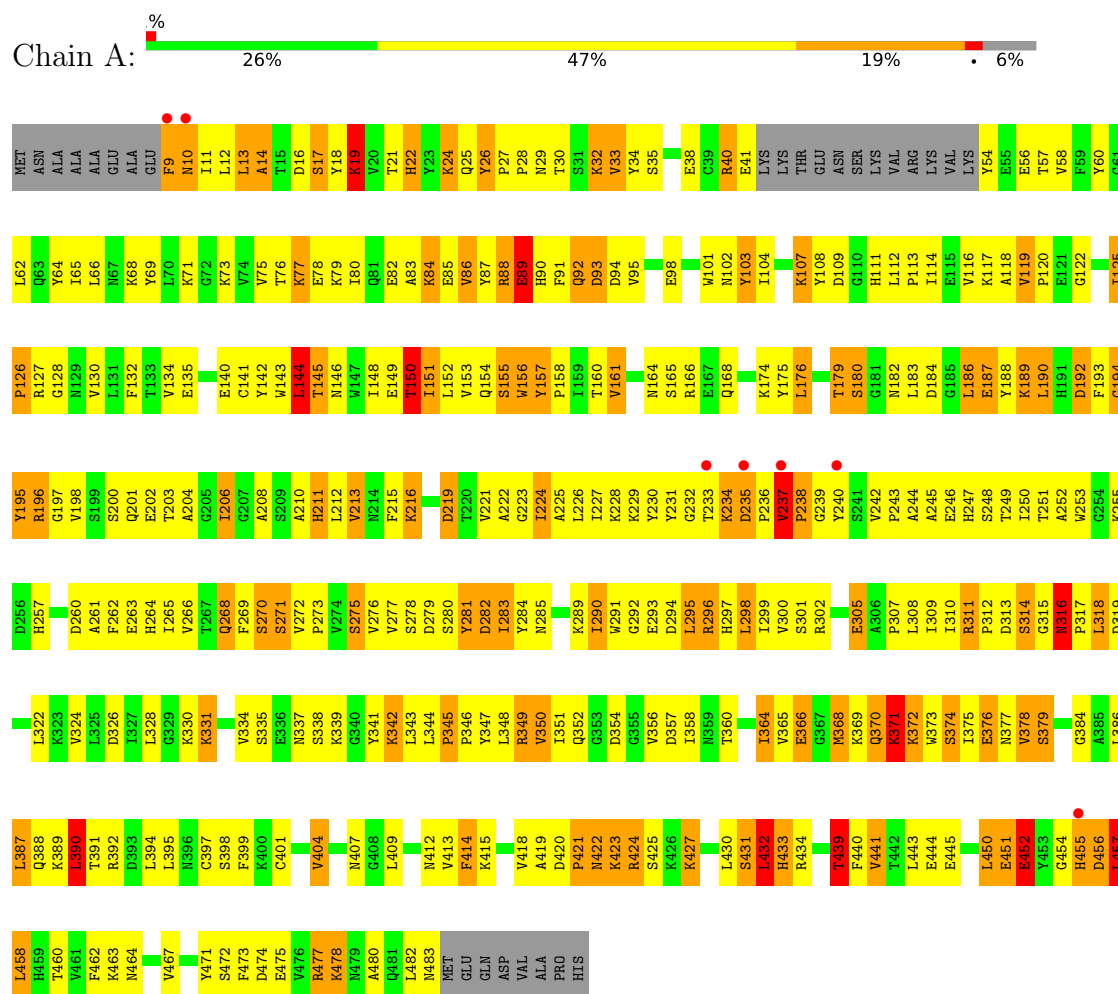
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	491	26% 47% 19% • 6%
1	B	491	30% 43% 19% • 6%

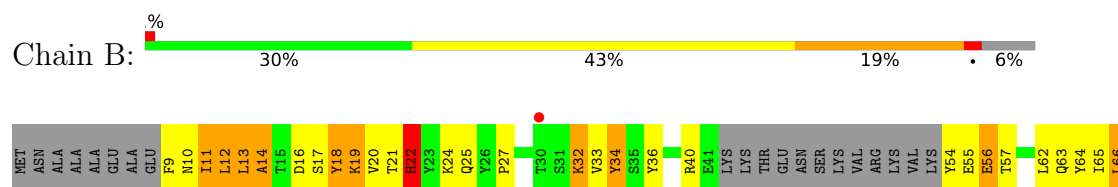
3 Residue-property plots

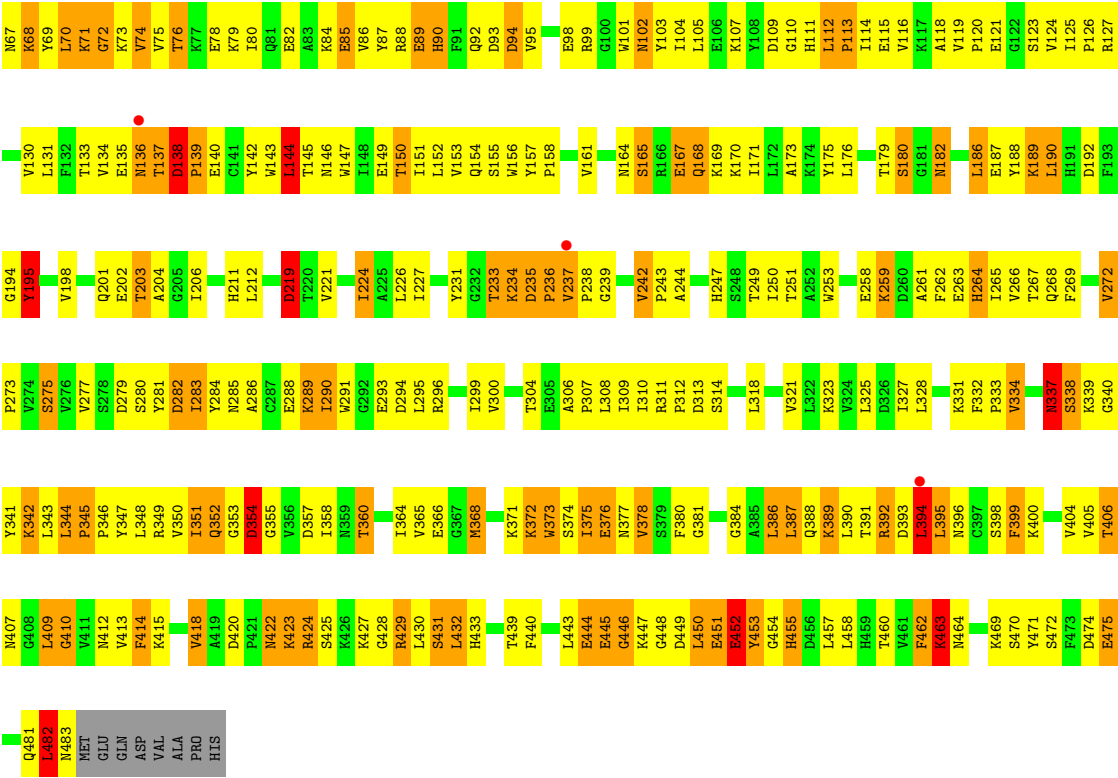
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Nicotinamide phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 107.41Å 120.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 98.8 (15.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.91 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.299 0.269 , 0.282	Depositor DCC
R_{free} test set	1136 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7476	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6152e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IS1

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	0.66	3/3788 (0.1%)	1.24	59/5136 (1.1%)
1	B	0.56	0/3788	1.19	45/5136 (0.9%)
All	All	0.61	3/7576 (0.0%)	1.21	104/10272 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	LEU	C-O	-10.94	1.11	1.24
1	A	457	LEU	CG-CD1	-8.69	1.23	1.52
1	A	432	LEU	CA-C	-5.09	1.46	1.52

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	SER	N-CA-C	-12.35	96.38	111.33
1	A	26	TYR	CA-C-N	-9.38	110.72	120.38
1	A	26	TYR	C-N-CA	-9.38	110.72	120.38
1	B	234	LYS	N-CA-C	-9.09	102.20	113.38
1	A	89	GLU	N-CA-C	-8.97	101.45	111.14
1	A	290	ILE	N-CA-C	8.95	119.76	110.72
1	A	201	GLN	N-CA-C	-8.76	101.03	112.68
1	A	86	VAL	N-CA-C	-8.44	103.54	111.48
1	A	84	LYS	N-CA-C	-8.16	99.80	110.33
1	A	423	LYS	N-CA-C	-7.95	103.37	113.23
1	B	74	VAL	N-CA-C	7.80	120.67	113.10
1	B	422	ASN	N-CA-C	-7.57	102.98	112.90
1	A	284	TYR	N-CA-C	-7.40	105.16	114.56
1	B	450	LEU	N-CA-C	-7.37	97.67	109.39
1	B	345	PRO	CA-C-N	7.37	129.05	119.84
1	B	345	PRO	C-N-CA	7.37	129.05	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ALA	N-CA-C	-7.35	102.55	112.26
1	B	289	LYS	N-CA-C	7.32	119.04	111.14
1	A	370	GLN	N-CA-C	-7.31	103.83	112.89
1	A	268	GLN	N-CA-C	-7.20	103.03	111.03
1	A	455	HIS	N-CA-C	7.06	125.84	110.80
1	A	103	TYR	N-CA-C	-7.01	102.69	111.11
1	B	482	LEU	N-CA-C	6.99	121.25	110.42
1	B	89	GLU	N-CA-C	-6.99	104.57	113.23
1	B	285	ASN	N-CA-C	-6.86	103.89	111.36
1	A	40	ARG	N-CA-C	6.74	120.25	110.42
1	A	155	SER	N-CA-C	-6.73	105.23	113.50
1	A	432	LEU	CA-C-O	-6.72	113.27	120.46
1	A	235	ASP	CA-C-N	6.71	128.22	119.84
1	A	235	ASP	C-N-CA	6.71	128.22	119.84
1	B	194	GLY	N-CA-C	6.69	122.00	113.24
1	A	156	TRP	N-CA-C	-6.68	103.65	112.34
1	B	373	TRP	N-CA-C	6.58	122.39	113.97
1	B	284	TYR	N-CA-C	-6.51	105.91	114.31
1	A	38	GLU	N-CA-C	6.50	117.04	107.88
1	B	14	ALA	N-CA-C	-6.48	102.67	110.44
1	B	392	ARG	N-CA-C	-6.46	104.66	112.54
1	B	138	ASP	CA-C-N	6.44	127.89	119.84
1	B	138	ASP	C-N-CA	6.44	127.89	119.84
1	A	311	ARG	N-CA-C	6.41	122.97	108.74
1	B	259	LYS	N-CA-C	6.41	119.26	111.82
1	A	140	GLU	N-CA-C	-6.35	105.69	113.50
1	B	290	ILE	N-CA-C	6.35	116.50	110.53
1	B	454	GLY	N-CA-C	-6.32	103.86	112.52
1	A	298	LEU	N-CA-C	-6.29	105.66	113.15
1	A	211	HIS	N-CA-C	-6.28	105.27	113.12
1	B	394	LEU	N-CA-C	-6.24	99.85	109.76
1	B	280	SER	N-CA-C	-6.21	104.20	110.97
1	A	345	PRO	CA-C-N	6.16	127.54	119.84
1	A	345	PRO	C-N-CA	6.16	127.54	119.84
1	A	460	THR	N-CA-C	-6.14	100.50	110.20
1	B	247	HIS	N-CA-C	6.07	119.95	112.54
1	A	313	ASP	N-CA-C	-6.03	100.48	109.83
1	B	448	GLY	N-CA-C	-5.99	107.76	114.40
1	B	56	GLU	N-CA-C	-5.96	98.10	110.80
1	B	112	LEU	CA-C-N	-5.95	112.40	119.84
1	B	112	LEU	C-N-CA	-5.95	112.40	119.84
1	A	144	LEU	N-CA-C	5.89	117.37	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	PRO	N-CA-C	5.89	121.71	113.53
1	B	267	THR	N-CA-C	-5.89	106.01	113.43
1	A	378	VAL	N-CA-C	5.83	117.14	108.46
1	B	462	PHE	N-CA-C	5.81	122.08	114.75
1	B	32	LYS	N-CA-C	5.78	117.81	108.34
1	B	90	HIS	N-CA-C	-5.76	104.64	111.03
1	A	350	VAL	N-CA-C	5.75	118.13	108.81
1	A	125	ILE	N-CA-C	5.66	114.73	108.05
1	B	68	LYS	N-CA-C	-5.63	106.45	113.38
1	B	334	VAL	N-CA-C	5.63	116.69	108.58
1	A	452	GLU	N-CA-C	-5.63	104.62	112.45
1	B	22	HIS	N-CA-C	5.62	122.77	110.80
1	A	364	ILE	N-CA-C	5.61	115.70	110.42
1	A	390	LEU	N-CA-C	-5.61	99.52	109.06
1	A	128	GLY	N-CA-C	-5.56	107.59	115.43
1	B	475	GLU	N-CA-C	-5.56	105.14	111.14
1	A	176	LEU	N-CA-C	-5.53	104.94	110.97
1	A	127	ARG	N-CA-C	5.45	118.94	110.17
1	A	281	TYR	N-CA-C	-5.43	100.92	109.50
1	B	12	LEU	N-CA-C	-5.42	106.64	113.20
1	A	433	HIS	N-CA-C	5.42	118.11	110.14
1	B	264	HIS	N-CA-C	-5.42	106.17	112.89
1	A	280	SER	N-CA-C	-5.41	105.30	111.14
1	A	285	ASN	N-CA-C	-5.40	104.94	112.45
1	B	219	ASP	N-CA-C	-5.38	106.08	113.30
1	A	22	HIS	N-CA-C	5.38	118.63	111.75
1	B	272	VAL	CA-C-N	-5.35	114.27	119.78
1	B	272	VAL	C-N-CA	-5.35	114.27	119.78
1	A	92	GLN	N-CA-C	-5.35	104.01	111.39
1	A	213	VAL	N-CA-C	-5.34	104.56	112.04
1	A	276	VAL	N-CA-C	5.34	115.68	107.77
1	A	439	THR	N-CA-C	5.28	122.04	110.80
1	B	144	LEU	N-CA-C	5.27	116.71	111.07
1	A	314	SER	N-CA-C	5.20	121.87	110.80
1	B	337	ASN	N-CA-C	5.18	116.69	108.96
1	A	237	VAL	CA-C-N	5.16	124.78	119.05
1	A	237	VAL	C-N-CA	5.16	124.78	119.05
1	A	371	LYS	N-CA-C	-5.16	106.83	113.23
1	A	427	LYS	N-CA-C	5.14	117.78	109.40
1	B	453	TYR	N-CA-C	-5.13	106.14	114.09
1	B	189	LYS	N-CA-C	5.12	119.51	113.16
1	A	356	VAL	N-CA-C	5.07	115.15	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	VAL	N-CA-C	-5.05	105.58	110.42
1	B	378	VAL	N-CA-C	5.04	116.56	108.89
1	A	19	LYS	CA-CB-CG	-5.01	104.09	114.10
1	A	450	LEU	N-CA-C	-5.01	98.44	107.75

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	3700	0	3665	424	0
1	B	3700	0	3665	403	0
2	A	38	0	37	15	0
2	B	38	0	37	8	0
All	All	7476	0	7404	792	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 53.

All (792) 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:432:LEU:O	1:A:457:LEU:CD1	1.90	1.19
1:A:19:LYS:HG3	1:A:22:HIS:CD2	1.80	1.15
1:A:432:LEU:O	1:A:457:LEU:HD13	1.46	1.12
1:A:148:ILE:HD13	1:A:152:LEU:HD12	1.32	1.11
1:B:179:THR:HG21	1:B:374:SER:HA	1.13	1.08
1:B:32:LYS:HD3	1:B:136:ASN:HD21	1.17	1.07
1:B:179:THR:CG2	1:B:374:SER:HA	1.86	1.04
1:A:13:LEU:HA	1:A:87:TYR:OH	1.56	1.04
1:B:391:THR:HG22	1:B:393:ASP:H	1.17	1.03
1:A:224:ILE:HG22	1:A:238:PRO:HG2	1.40	1.02
1:A:104:ILE:HD11	1:A:141:CYS:SG	2.03	0.99
1:A:224:ILE:CG2	1:A:238:PRO:HG2	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:HIS:HA	1:A:457:LEU:HD11	1.45	0.97
1:A:316:ASN:ND2	1:A:319:ASP:H	1.62	0.96
1:B:112:LEU:HD22	1:B:144:LEU:HD11	1.46	0.96
1:B:311:ARG:HG3	1:B:351:ILE:HG23	1.48	0.96
1:B:149:GLU:HG3	1:B:399:PHE:CD2	2.01	0.95
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.49	0.95
1:B:175:TYR:OH	1:B:366:GLU:HG2	1.67	0.95
1:B:482:LEU:HD23	1:B:483:ASN:H	1.28	0.94
1:A:179:THR:CG2	1:A:374:SER:HA	1.97	0.94
1:B:405:VAL:HA	1:B:410:GLY:HA2	1.51	0.93
1:A:151:ILE:HD12	1:B:201:GLN:HE21	1.33	0.93
1:A:179:THR:HG21	1:A:375:ILE:H	1.34	0.93
1:A:193:PHE:HD2	2:A:501:IS1:H2'	1.35	0.92
1:A:212:LEU:HD12	1:A:227:ILE:HD11	1.53	0.91
1:B:198:VAL:HG21	1:B:204:ALA:HB2	1.52	0.91
1:A:10:ASN:HB3	1:A:13:LEU:HD11	1.50	0.90
1:A:148:ILE:HD13	1:A:152:LEU:CD1	2.01	0.89
1:B:337:ASN:HD22	1:B:339:LYS:H	1.13	0.89
1:B:198:VAL:HG11	1:B:387:LEU:HD12	1.55	0.89
1:B:179:THR:HG21	1:B:374:SER:CA	2.02	0.89
1:A:202:GLU:O	1:A:206:ILE:HD13	1.71	0.88
1:B:374:SER:OG	1:B:376:GLU:HG3	1.73	0.88
1:B:337:ASN:ND2	1:B:339:LYS:H	1.71	0.87
1:B:309:ILE:HD13	1:B:349:ARG:HB2	1.55	0.87
1:B:311:ARG:HH11	2:B:502:IS1:HAG	1.40	0.87
1:A:32:LYS:NZ	1:A:135:GLU:OE1	2.08	0.86
1:A:198:VAL:HG21	1:A:204:ALA:HB2	1.55	0.86
1:B:325:LEU:HD11	1:B:368:MET:HE3	1.58	0.86
1:A:149:GLU:HG3	1:A:399:PHE:CD2	2.11	0.86
1:A:10:ASN:HB3	1:A:13:LEU:CD1	2.06	0.86
1:B:71:LYS:HE3	1:B:72:GLY:H	1.42	0.85
1:B:13:LEU:HA	1:B:87:TYR:OH	1.76	0.85
1:A:193:PHE:CD2	2:A:501:IS1:H2'	2.10	0.85
1:B:13:LEU:N	1:B:13:LEU:HD22	1.92	0.85
1:B:80:ILE:HG21	1:B:102:ASN:HD21	1.42	0.85
1:A:9:PHE:O	1:A:10:ASN:HB2	1.77	0.84
1:B:113:PRO:C	1:B:137:THR:HG1	1.85	0.84
1:B:309:ILE:CD1	1:B:349:ARG:HB2	2.08	0.83
1:A:432:LEU:O	1:A:457:LEU:HD12	1.77	0.83
1:B:155:SER:O	1:B:158:PRO:HD2	1.79	0.83
1:B:32:LYS:HD3	1:B:136:ASN:ND2	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG12	1:A:375:ILE:HD12	1.60	0.83
1:B:13:LEU:HD22	1:B:13:LEU:H	1.43	0.83
1:A:421:PRO:C	1:A:423:LYS:H	1.87	0.83
1:A:243:PRO:HA	1:B:21:THR:HG21	1.61	0.82
1:A:388:GLN:HG3	1:A:389:LYS:H	1.44	0.82
1:A:84:LYS:O	1:A:85:GLU:HB3	1.78	0.82
1:A:326:ASP:O	1:A:330:LYS:HG3	1.78	0.82
1:B:405:VAL:HA	1:B:410:GLY:CA	2.08	0.82
1:B:113:PRO:HB2	1:B:137:THR:OG1	1.79	0.82
1:A:374:SER:HB3	1:A:376:GLU:HG3	1.62	0.82
1:B:323:LYS:O	1:B:327:ILE:HD13	1.80	0.81
1:A:175:TYR:OH	1:A:366:GLU:HG2	1.81	0.81
1:A:98:GLU:O	1:A:102:ASN:ND2	2.13	0.81
1:A:463:LYS:HG3	1:A:464:ASN:ND2	1.96	0.81
1:A:77:LYS:HE2	1:A:77:LYS:H	1.46	0.80
1:A:179:THR:HG23	1:A:374:SER:HA	1.60	0.80
1:A:10:ASN:CB	1:A:13:LEU:HD11	2.10	0.80
1:B:237:VAL:HG12	1:B:237:VAL:O	1.82	0.80
1:A:149:GLU:O	1:A:153:VAL:HG23	1.82	0.79
1:A:151:ILE:HD12	1:B:201:GLN:NE2	1.98	0.79
1:B:54:TYR:OH	1:B:164:ASN:ND2	2.16	0.79
1:B:32:LYS:HE2	1:B:135:GLU:HG3	1.65	0.78
1:A:206:ILE:HD12	1:A:226:LEU:CD1	2.14	0.78
1:A:12:LEU:HD11	1:A:80:ILE:HD13	1.64	0.78
1:A:272:VAL:HB	1:A:273:PRO:CD	2.14	0.77
2:A:501:IS1:CAM	2:A:501:IS1:HAXA	2.14	0.77
1:B:355:GLY:O	1:B:360:THR:HG21	1.85	0.77
1:B:93:ASP:OD1	1:B:94:ASP:N	2.18	0.77
1:B:71:LYS:HE3	1:B:72:GLY:N	1.99	0.77
1:A:19:LYS:CG	1:A:22:HIS:CD2	2.67	0.75
1:A:379:SER:HB3	2:A:501:IS1:CAI	2.16	0.75
1:A:112:LEU:HD22	1:A:144:LEU:HD11	1.67	0.75
1:B:308:LEU:HD21	1:B:310:ILE:HD11	1.69	0.75
1:B:482:LEU:HD23	1:B:483:ASN:N	2.01	0.75
1:B:156:TRP:CG	1:B:392:ARG:HG3	2.22	0.75
1:A:234:LYS:N	1:A:234:LYS:HD2	2.02	0.75
1:A:57:THR:HG22	1:A:395:LEU:HD13	1.69	0.74
1:B:57:THR:CG2	1:B:395:LEU:HD13	2.17	0.74
1:B:161:VAL:O	1:B:165:SER:HB2	1.85	0.74
1:A:224:ILE:HG22	1:A:238:PRO:CG	2.15	0.74
1:B:157:TYR:HB3	1:B:158:PRO:HD3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LYS:HG3	1:B:372:LYS:O	1.87	0.74
1:A:179:THR:HG21	1:A:374:SER:HA	1.70	0.73
1:B:103:TYR:CZ	1:B:140:GLU:HG3	2.23	0.73
1:A:316:ASN:HD21	1:A:319:ASP:H	1.35	0.73
1:B:311:ARG:NH1	2:B:502:IS1:HAG	2.02	0.73
1:B:450:LEU:O	1:B:452:GLU:HG2	1.88	0.73
1:A:343:LEU:HD12	1:A:377:ASN:OD1	1.88	0.73
1:B:296:ARG:NH1	1:B:331:LYS:O	2.22	0.73
1:B:413:VAL:O	1:B:414:PHE:HB3	1.89	0.72
1:B:165:SER:OG	1:B:211:HIS:HD2	1.71	0.72
1:A:251:THR:HG22	1:A:281:TYR:OH	1.89	0.72
1:A:145:THR:O	1:A:148:ILE:HG13	1.88	0.72
1:A:179:THR:HG21	1:A:375:ILE:N	2.03	0.72
1:B:153:VAL:C	1:B:155:SER:H	1.98	0.72
1:B:113:PRO:O	1:B:137:THR:OG1	2.07	0.72
1:A:119:VAL:HG11	1:A:125:ILE:HD11	1.71	0.72
1:A:349:ARG:HG2	1:A:349:ARG:HH11	1.54	0.72
1:A:457:LEU:HD12	1:A:457:LEU:N	2.04	0.72
1:A:168:GLN:HG3	1:A:358:ILE:HD13	1.69	0.71
1:B:104:ILE:HD12	1:B:104:ILE:H	1.53	0.71
1:A:76:THR:OG1	1:A:79:LYS:HG3	1.90	0.71
1:A:10:ASN:CG	1:A:13:LEU:HD11	2.14	0.71
1:A:157:TYR:HB3	1:A:158:PRO:HD3	1.71	0.71
1:B:373:TRP:O	1:B:374:SER:HB3	1.90	0.71
1:B:398:SER:OG	1:B:400:LYS:HE3	1.92	0.70
1:A:433:HIS:HA	1:A:457:LEU:CD1	2.19	0.70
1:B:337:ASN:HD22	1:B:337:ASN:C	1.98	0.70
1:A:316:ASN:ND2	1:A:319:ASP:N	2.37	0.70
1:B:429:ARG:NH1	1:B:446:GLY:HA3	2.07	0.69
1:B:439:THR:HG23	1:B:440:PHE:N	2.06	0.69
1:A:13:LEU:HA	1:A:87:TYR:HH	1.55	0.69
1:B:82:GLU:O	1:B:86:VAL:HG23	1.91	0.69
1:B:113:PRO:C	1:B:137:THR:OG1	2.35	0.69
1:B:180:SER:HB2	1:B:376:GLU:OE1	1.92	0.69
1:B:71:LYS:HG2	1:B:72:GLY:H	1.57	0.69
1:A:182:ASN:HD22	1:A:184:ASP:H	1.38	0.69
1:A:421:PRO:O	1:A:423:LYS:N	2.26	0.69
1:B:10:ASN:HB3	1:B:13:LEU:HD21	1.73	0.69
1:B:263:GLU:HA	1:B:266:VAL:HG22	1.75	0.69
1:A:76:THR:HG23	1:A:79:LYS:HE3	1.76	0.68
1:A:14:ALA:HA	1:B:195:TYR:OH	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:VAL:HG12	1:B:414:PHE:N	2.09	0.68
1:A:120:PRO:HA	1:A:471:TYR:CZ	2.29	0.68
1:A:349:ARG:HG2	1:A:349:ARG:NH1	2.06	0.68
1:B:165:SER:OG	1:B:211:HIS:CD2	2.47	0.68
1:A:54:TYR:OH	1:A:164:ASN:ND2	2.26	0.68
1:A:263:GLU:HG3	1:A:298:LEU:CD1	2.23	0.68
1:A:176:LEU:HD22	1:A:182:ASN:O	1.94	0.67
1:A:431:SER:HB2	1:A:433:HIS:NE2	2.09	0.67
1:B:415:LYS:H	1:B:425:SER:HB3	1.57	0.67
1:A:299:ILE:HG23	1:A:300:VAL:H	1.59	0.67
1:A:311:ARG:HG3	1:A:351:ILE:HG13	1.76	0.67
1:B:374:SER:OG	1:B:376:GLU:CG	2.42	0.67
1:A:89:GLU:OE2	1:B:238:PRO:HD2	1.94	0.67
1:B:56:GLU:O	1:B:56:GLU:HG3	1.94	0.67
1:B:71:LYS:CG	1:B:72:GLY:H	2.05	0.67
1:A:86:VAL:C	1:A:88:ARG:H	2.01	0.67
1:B:353:GLY:HA2	1:B:381:GLY:O	1.94	0.67
1:B:264:HIS:O	1:B:268:GLN:HG2	1.94	0.67
1:B:182:ASN:C	1:B:182:ASN:HD22	2.03	0.66
1:A:17:SER:OG	1:A:90:HIS:HE1	1.78	0.66
1:A:122:GLY:O	1:A:480:ALA:HB2	1.95	0.66
1:A:257:HIS:ND1	1:A:260:ASP:OD2	2.28	0.66
1:B:123:SER:HB3	1:B:125:ILE:CD1	2.25	0.66
1:B:78:GLU:OE1	1:B:78:GLU:N	2.27	0.66
1:A:374:SER:CB	1:A:376:GLU:HG3	2.24	0.66
1:B:431:SER:HB2	1:B:433:HIS:NE2	2.10	0.66
1:A:189:LYS:NZ	1:A:376:GLU:HA	2.11	0.66
1:A:118:ALA:O	1:A:458:LEU:HA	1.94	0.66
1:A:252:ALA:O	1:B:27:PRO:HG3	1.96	0.66
1:B:311:ARG:NH1	2:B:502:IS1:CAG	2.59	0.66
1:B:57:THR:HG22	1:B:395:LEU:HD13	1.78	0.66
1:B:80:ILE:HD12	1:B:101:TRP:HB3	1.78	0.66
1:B:123:SER:HB3	1:B:125:ILE:HD11	1.77	0.65
1:A:221:VAL:HG21	1:B:13:LEU:HB2	1.78	0.65
1:B:151:ILE:HG23	1:B:152:LEU:N	2.11	0.65
1:A:463:LYS:HG3	1:A:464:ASN:HD22	1.60	0.65
1:A:179:THR:CG2	1:A:375:ILE:H	2.08	0.64
1:B:386:LEU:HD13	1:B:387:LEU:HD23	1.79	0.64
1:B:136:ASN:OD1	1:B:142:TYR:HA	1.97	0.64
1:B:325:LEU:CD1	1:B:368:MET:HE3	2.28	0.64
1:B:413:VAL:CG1	1:B:414:PHE:N	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:HG12	1:B:387:LEU:HB3	1.78	0.64
1:A:9:PHE:HD2	1:A:9:PHE:N	1.96	0.64
1:A:264:HIS:O	1:A:268:GLN:HG2	1.96	0.64
1:A:299:ILE:HG23	1:A:300:VAL:N	2.13	0.64
1:B:289:LYS:HA	1:B:293:GLU:HG3	1.80	0.64
1:A:148:ILE:CD1	1:A:152:LEU:HD12	2.20	0.64
1:A:412:ASN:ND2	1:A:445:GLU:HG2	2.13	0.64
1:A:243:PRO:CA	1:B:21:THR:HG21	2.28	0.63
1:B:155:SER:C	1:B:158:PRO:HD2	2.23	0.63
1:B:56:GLU:HA	1:B:126:PRO:HA	1.80	0.63
1:B:296:ARG:HA	1:B:299:ILE:HD12	1.79	0.63
1:A:206:ILE:HD12	1:A:226:LEU:HD11	1.79	0.63
1:B:198:VAL:HB	1:B:203:THR:CG2	2.29	0.63
1:A:221:VAL:O	1:A:224:ILE:HG13	1.98	0.63
1:A:153:VAL:C	1:A:155:SER:H	2.06	0.63
1:B:70:LEU:HD21	1:B:151:ILE:HG21	1.79	0.63
1:B:86:VAL:C	1:B:88:ARG:H	2.07	0.63
1:B:113:PRO:CB	1:B:137:THR:OG1	2.45	0.63
1:A:420:ASP:OD2	1:A:423:LYS:HG3	1.98	0.63
1:B:116:VAL:HG13	1:B:134:VAL:HG22	1.79	0.63
1:B:283:ILE:CD1	1:B:312:PRO:HA	2.28	0.63
1:A:342:LYS:HZ2	1:A:342:LYS:CB	2.12	0.62
1:A:80:ILE:HD12	1:A:101:TRP:HB3	1.79	0.62
1:B:114:ILE:CA	1:B:137:THR:HG23	2.29	0.62
1:B:304:THR:HG22	1:B:346:PRO:HB2	1.81	0.62
1:A:195:TYR:OH	1:B:14:ALA:HA	2.00	0.62
1:B:73:LYS:HG3	1:B:109:ASP:O	1.99	0.62
1:B:149:GLU:HG3	1:B:399:PHE:CE2	2.35	0.62
1:B:167:GLU:O	1:B:170:LYS:N	2.32	0.62
1:B:351:ILE:HD13	1:B:352:GLN:N	2.14	0.62
1:B:237:VAL:O	1:B:237:VAL:CG1	2.47	0.62
1:A:156:TRP:HH2	1:B:388:GLN:HE21	1.48	0.62
1:A:84:LYS:C	1:A:86:VAL:H	2.08	0.61
1:B:24:LYS:NZ	1:B:95:VAL:HG12	2.15	0.61
1:A:212:LEU:HD12	1:A:227:ILE:CD1	2.26	0.61
1:B:136:ASN:C	1:B:136:ASN:HD22	2.07	0.61
1:A:156:TRP:CB	1:A:392:ARG:HG3	2.30	0.61
1:B:75:VAL:CG1	1:B:80:ILE:HD11	2.30	0.61
1:B:198:VAL:CG1	1:B:387:LEU:HB3	2.31	0.61
1:A:300:VAL:HG13	1:A:347:TYR:CE2	2.34	0.61
1:B:311:ARG:HG3	1:B:351:ILE:CG2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PHE:CD2	2:A:501:IS1:C2'	2.82	0.61
1:B:413:VAL:CG1	1:B:414:PHE:H	2.13	0.61
1:A:432:LEU:CB	1:A:458:LEU:HD21	2.31	0.61
1:B:337:ASN:HD22	1:B:339:LYS:N	1.92	0.61
1:B:337:ASN:O	1:B:340:GLY:N	2.32	0.61
1:B:70:LEU:O	1:B:71:LYS:O	2.18	0.61
1:B:373:TRP:O	1:B:377:ASN:ND2	2.34	0.60
1:A:148:ILE:HD12	1:A:148:ILE:C	2.25	0.60
1:A:414:PHE:N	1:A:414:PHE:CD2	2.69	0.60
1:A:433:HIS:CD2	1:A:443:LEU:HD12	2.36	0.60
1:A:432:LEU:HB2	1:A:458:LEU:HD21	1.83	0.60
1:A:9:PHE:N	1:A:9:PHE:CD2	2.69	0.60
1:A:12:LEU:CD1	1:A:80:ILE:HD13	2.30	0.60
1:B:127:ARG:CZ	1:B:395:LEU:HA	2.32	0.60
1:B:24:LYS:HZ1	1:B:95:VAL:HG12	1.66	0.60
1:B:445:GLU:C	1:B:447:LYS:H	2.09	0.60
1:A:12:LEU:O	1:A:87:TYR:CE1	2.55	0.60
2:A:501:IS1:O2'	2:A:501:IS1:HAP	2.01	0.60
1:B:272:VAL:C	1:B:306:ALA:HB1	2.27	0.60
1:B:273:PRO:HG3	1:B:306:ALA:HA	1.84	0.60
1:B:350:VAL:HB	1:B:378:VAL:HG22	1.83	0.60
1:A:373:TRP:O	1:A:374:SER:C	2.44	0.60
1:B:233:THR:HG22	1:B:235:ASP:HB2	1.82	0.60
1:B:180:SER:HB2	1:B:376:GLU:CD	2.27	0.59
1:A:19:LYS:C	1:A:21:THR:N	2.57	0.59
1:B:399:PHE:CD2	1:B:399:PHE:C	2.81	0.59
1:A:316:ASN:C	1:A:316:ASN:HD22	2.10	0.59
1:B:365:VAL:HG12	1:B:375:ILE:HD12	1.85	0.59
1:A:272:VAL:HB	1:A:273:PRO:HD2	1.83	0.59
1:B:13:LEU:HA	1:B:87:TYR:HH	1.63	0.59
1:B:395:LEU:HD23	1:B:395:LEU:N	2.17	0.59
1:B:12:LEU:HD21	1:B:80:ILE:HD13	1.85	0.59
1:A:237:VAL:HG21	1:B:89:GLU:HB3	1.85	0.58
1:B:13:LEU:N	1:B:13:LEU:CD2	2.64	0.58
1:B:313:ASP:CG	1:B:313:ASP:O	2.46	0.58
1:A:9:PHE:CE2	1:A:69:TYR:HD2	2.21	0.58
1:B:134:VAL:HG21	1:B:152:LEU:CD1	2.33	0.58
1:A:80:ILE:CD1	1:A:101:TRP:HB3	2.33	0.58
1:B:332:PHE:HB3	1:B:333:PRO:HD2	1.85	0.58
1:B:337:ASN:ND2	1:B:337:ASN:C	2.61	0.58
1:A:21:THR:HG21	1:B:243:PRO:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:HG3	1:A:389:LYS:N	2.16	0.58
1:A:414:PHE:HB2	1:A:425:SER:HB2	1.85	0.58
1:B:57:THR:HG21	1:B:395:LEU:HD13	1.84	0.58
1:A:309:ILE:CD1	1:A:349:ARG:HB2	2.33	0.58
1:B:32:LYS:O	1:B:404:VAL:HA	2.04	0.58
1:A:73:LYS:HG3	1:A:109:ASP:O	2.03	0.58
1:A:348:LEU:O	1:A:349:ARG:HG2	2.04	0.58
1:A:414:PHE:N	1:A:414:PHE:HD2	2.02	0.58
1:B:179:THR:CG2	1:B:374:SER:CA	2.73	0.58
1:B:300:VAL:HG13	1:B:347:TYR:CZ	2.39	0.57
1:A:87:TYR:CE2	1:B:221:VAL:HG11	2.40	0.57
1:B:138:ASP:OD2	1:B:138:ASP:C	2.47	0.57
1:A:427:LYS:HZ3	1:A:427:LYS:HB2	1.69	0.57
1:A:75:VAL:CG1	1:A:80:ILE:HD11	2.34	0.57
1:A:224:ILE:HA	1:A:227:ILE:HD12	1.86	0.57
1:A:473:PHE:O	1:A:477:ARG:HG2	2.04	0.57
1:A:212:LEU:HA	1:A:215:PHE:O	2.04	0.57
1:B:167:GLU:O	1:B:169:LYS:N	2.37	0.57
1:B:318:LEU:HB2	1:B:364:ILE:HD13	1.86	0.57
1:A:76:THR:CG2	1:A:79:LYS:HE3	2.33	0.57
1:A:318:LEU:HA	1:A:364:ILE:HD12	1.86	0.57
1:B:202:GLU:O	1:B:206:ILE:HG13	2.04	0.57
1:B:286:ALA:HA	1:B:290:ILE:HD12	1.87	0.57
1:A:9:PHE:CZ	1:A:69:TYR:HD2	2.23	0.57
1:A:357:ASP:OD2	1:A:360:THR:HB	2.05	0.57
1:A:413:VAL:HG13	1:B:251:THR:HB	1.87	0.57
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.19	0.56
1:A:235:ASP:HB3	1:A:236:PRO:HD2	1.87	0.56
1:A:12:LEU:O	1:A:87:TYR:HE1	1.87	0.56
1:A:242:VAL:HG22	2:A:501:IS1:HATA	1.88	0.56
1:B:84:LYS:HE3	1:B:98:GLU:OE1	2.05	0.56
1:A:28:PRO:O	1:A:29:ASN:HB2	2.04	0.56
1:A:193:PHE:HD2	2:A:501:IS1:C2'	2.14	0.56
1:A:292:GLY:C	1:A:293:GLU:HG2	2.29	0.56
1:A:374:SER:C	1:A:376:GLU:H	2.14	0.56
1:B:63:GLN:OE1	1:B:470:SER:HA	2.06	0.56
1:B:450:LEU:O	1:B:451:GLU:C	2.47	0.56
1:A:189:LYS:HE2	1:A:378:VAL:O	2.05	0.56
1:A:371:LYS:O	1:A:372:LYS:HB2	2.05	0.56
1:A:309:ILE:HD13	1:A:349:ARG:HB2	1.88	0.56
1:B:115:GLU:HG3	1:B:463:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:HG23	1:B:283:ILE:O	2.04	0.56
1:B:80:ILE:CD1	1:B:101:TRP:HB3	2.36	0.56
1:B:149:GLU:O	1:B:153:VAL:HG23	2.06	0.56
1:B:373:TRP:O	1:B:374:SER:CB	2.51	0.56
1:B:242:VAL:HG22	2:B:502:IS1:HATA	1.88	0.56
1:B:262:PHE:O	1:B:266:VAL:HG22	2.05	0.56
1:A:300:VAL:HG13	1:A:347:TYR:CZ	2.41	0.55
1:A:472:SER:C	1:A:474:ASP:H	2.14	0.55
1:B:146:ASN:O	1:B:147:TRP:C	2.48	0.55
1:B:353:GLY:O	1:B:354:ASP:CB	2.55	0.55
1:B:114:ILE:N	1:B:137:THR:HG23	2.22	0.55
1:A:160:THR:HG23	1:A:394:LEU:HD23	1.87	0.55
1:A:277:VAL:O	1:A:277:VAL:HG23	2.07	0.55
1:B:186:LEU:O	1:B:188:TYR:N	2.40	0.55
1:A:25:GLN:HB2	1:B:249:THR:HB	1.89	0.55
1:A:224:ILE:O	1:A:225:ALA:C	2.50	0.55
1:A:418:VAL:HG13	1:A:419:ALA:N	2.21	0.55
1:B:136:ASN:ND2	1:B:136:ASN:C	2.63	0.55
1:B:142:TYR:CD1	1:B:143:TRP:N	2.75	0.55
1:B:198:VAL:HB	1:B:203:THR:HG22	1.88	0.55
1:B:424:ARG:HG2	1:B:425:SER:H	1.72	0.55
1:B:231:TYR:O	1:B:472:SER:HA	2.07	0.55
1:A:57:THR:CG2	1:A:395:LEU:HD13	2.35	0.55
1:B:76:THR:O	1:B:80:ILE:HG12	2.06	0.55
1:B:151:ILE:CG2	1:B:152:LEU:N	2.69	0.55
1:B:406:THR:HG22	1:B:406:THR:O	2.07	0.55
1:A:144:LEU:O	1:A:145:THR:C	2.49	0.55
1:A:317:PRO:HB2	1:A:364:ILE:HD11	1.89	0.55
1:A:35:SER:HB3	1:A:399:PHE:CE2	2.42	0.55
1:A:208:ALA:O	1:A:212:LEU:HG	2.07	0.55
1:B:344:LEU:CB	1:B:345:PRO:HD2	2.37	0.54
1:A:175:TYR:O	1:A:179:THR:HB	2.07	0.54
1:B:71:LYS:HG2	1:B:72:GLY:N	2.23	0.54
1:B:404:VAL:O	1:B:410:GLY:HA2	2.07	0.54
1:B:472:SER:C	1:B:474:ASP:H	2.15	0.54
1:A:9:PHE:CZ	1:A:69:TYR:CD2	2.95	0.54
1:A:430:LEU:CD2	1:A:444:GLU:HG2	2.37	0.54
1:A:472:SER:OG	1:A:475:GLU:HG3	2.07	0.54
1:A:155:SER:C	1:A:157:TYR:N	2.58	0.54
1:A:27:PRO:HA	1:B:253:TRP:CZ2	2.43	0.54
1:A:93:ASP:OD1	1:A:94:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:O	1:A:239:GLY:HA2	2.08	0.54
1:A:263:GLU:OE1	1:A:295:LEU:HD11	2.07	0.54
1:A:315:GLY:O	1:A:316:ASN:HB3	2.06	0.54
1:B:409:LEU:HD22	1:B:409:LEU:H	1.72	0.54
1:A:316:ASN:ND2	1:A:316:ASN:C	2.66	0.54
1:B:68:LYS:NZ	1:B:69:TYR:CZ	2.76	0.54
1:B:173:ALA:HB2	1:B:186:LEU:HD11	1.90	0.54
1:B:371:LYS:O	1:B:372:LYS:HB2	2.08	0.54
1:A:282:ASP:HA	1:B:418:VAL:HG22	1.90	0.54
1:B:17:SER:OG	1:B:90:HIS:HE1	1.90	0.54
1:B:311:ARG:HH11	2:B:502:IS1:CAG	2.14	0.54
1:A:10:ASN:O	1:A:13:LEU:HD12	2.08	0.53
1:A:119:VAL:HG12	1:A:120:PRO:HD2	1.90	0.53
1:B:112:LEU:CD2	1:B:144:LEU:HD11	2.31	0.53
1:B:445:GLU:C	1:B:447:LYS:N	2.66	0.53
1:A:62:LEU:HD12	1:A:62:LEU:O	2.09	0.53
1:B:11:ILE:HD13	1:B:11:ILE:O	2.07	0.53
1:B:40:ARG:CG	1:B:400:LYS:HZ1	2.21	0.53
1:B:104:ILE:H	1:B:104:ILE:CD1	2.21	0.53
1:B:179:THR:HG23	1:B:341:TYR:CG	2.43	0.53
1:A:149:GLU:CG	1:A:399:PHE:CD2	2.90	0.53
1:B:333:PRO:O	1:B:345:PRO:HD3	2.08	0.53
1:A:432:LEU:C	1:A:457:LEU:HD13	2.23	0.53
1:A:198:VAL:HG11	1:A:387:LEU:HD12	1.90	0.53
1:B:146:ASN:O	1:B:149:GLU:N	2.24	0.53
1:B:321:VAL:CG2	1:B:352:GLN:HG3	2.38	0.53
1:A:418:VAL:C	1:A:420:ASP:H	2.16	0.53
1:A:296:ARG:C	1:A:299:ILE:HG22	2.34	0.53
1:A:297:HIS:C	1:A:299:ILE:H	2.15	0.53
1:B:105:LEU:HA	1:B:110:GLY:H	1.74	0.53
1:A:251:THR:HB	1:B:413:VAL:HG13	1.91	0.52
1:B:168:GLN:HA	1:B:171:ILE:HD13	1.91	0.52
1:B:263:GLU:HB2	1:B:295:LEU:HD22	1.91	0.52
1:A:211:HIS:HD2	1:A:386:LEU:HD11	1.73	0.52
1:A:261:ALA:O	1:A:262:PHE:C	2.52	0.52
1:A:318:LEU:CA	1:A:364:ILE:HD12	2.40	0.52
1:B:114:ILE:HG23	1:B:144:LEU:HD13	1.91	0.52
1:B:234:LYS:HD3	1:B:234:LYS:N	2.24	0.52
1:A:455:HIS:O	1:A:456:ASP:C	2.52	0.52
1:B:304:THR:HG22	1:B:346:PRO:CB	2.38	0.52
1:A:196:ARG:HH11	1:A:196:ARG:HB3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:C	1:A:301:SER:N	2.66	0.52
1:A:86:VAL:C	1:A:88:ARG:N	2.62	0.52
1:A:455:HIS:C	1:A:456:ASP:O	2.48	0.52
1:B:118:ALA:O	1:B:458:LEU:HA	2.08	0.52
1:B:398:SER:CB	1:B:400:LYS:HE3	2.39	0.52
1:A:281:TYR:O	1:A:282:ASP:C	2.53	0.52
1:A:413:VAL:CG1	1:A:414:PHE:N	2.72	0.52
1:B:190:LEU:O	1:B:211:HIS:HE1	1.93	0.52
1:B:391:THR:HG21	1:B:393:ASP:HB2	1.92	0.52
1:B:418:VAL:HG23	1:B:418:VAL:O	2.10	0.52
1:A:224:ILE:HG21	1:A:238:PRO:HG2	1.86	0.52
1:A:283:ILE:HD13	1:A:312:PRO:HB3	1.92	0.52
1:B:55:GLU:HA	1:B:127:ARG:HD3	1.91	0.52
1:A:368:MET:HE1	1:A:378:VAL:HB	1.91	0.52
1:B:328:LEU:HD13	1:B:348:LEU:HD11	1.91	0.52
1:A:17:SER:C	1:A:19:LYS:H	2.17	0.51
1:A:33:VAL:CG1	1:A:142:TYR:O	2.58	0.51
1:A:189:LYS:HG3	1:A:379:SER:HA	1.92	0.51
2:A:501:IS1:O2'	2:A:501:IS1:CAP	2.58	0.51
1:B:19:LYS:HG3	1:B:22:HIS:CD2	2.45	0.51
1:B:116:VAL:HG13	1:B:133:THR:O	2.10	0.51
1:A:82:GLU:O	1:A:86:VAL:HG23	2.10	0.51
1:B:198:VAL:HB	1:B:203:THR:HG21	1.93	0.51
1:A:32:LYS:O	1:A:404:VAL:HA	2.10	0.51
1:B:345:PRO:HB2	1:B:347:TYR:CZ	2.45	0.51
1:A:157:TYR:O	1:A:158:PRO:C	2.50	0.51
1:B:462:PHE:O	1:B:463:LYS:C	2.52	0.51
1:A:183:LEU:HD13	1:A:186:LEU:HD12	1.93	0.51
1:B:233:THR:C	1:B:234:LYS:HD3	2.35	0.51
1:A:242:VAL:HG11	2:A:501:IS1:HAW	1.92	0.51
1:A:375:ILE:HG22	1:A:375:ILE:O	2.09	0.51
1:A:130:VAL:CG1	1:A:432:LEU:HB2	2.40	0.51
1:A:175:TYR:HH	1:A:366:GLU:HG2	1.76	0.51
1:A:189:LYS:HZ1	1:A:376:GLU:HA	1.73	0.51
1:B:104:ILE:HD12	1:B:104:ILE:N	2.24	0.51
1:A:62:LEU:O	1:A:66:LEU:HG	2.10	0.51
1:A:161:VAL:O	1:A:165:SER:HB3	2.11	0.51
1:A:375:ILE:O	1:A:375:ILE:CG2	2.58	0.51
1:B:11:ILE:HG12	1:B:14:ALA:HB3	1.92	0.51
1:A:26:TYR:O	1:A:27:PRO:C	2.47	0.51
1:A:192:ASP:OD1	1:A:192:ASP:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:HD2	1:A:65:ILE:HG13	1.75	0.50
1:A:193:PHE:CD2	2:A:501:IS1:O2'	2.61	0.50
1:A:311:ARG:NH1	2:A:501:IS1:HAG	2.26	0.50
1:B:120:PRO:HA	1:B:471:TYR:CZ	2.46	0.50
1:B:171:ILE:HD12	1:B:171:ILE:H	1.76	0.50
1:B:388:GLN:HG3	1:B:389:LYS:H	1.75	0.50
1:A:73:LYS:HA	1:A:111:HIS:HD2	1.76	0.50
1:A:200:SER:OG	1:B:203:THR:OG1	2.26	0.50
1:A:68:LYS:O	1:A:68:LYS:HG2	2.10	0.50
1:A:283:ILE:HG12	1:A:283:ILE:O	2.12	0.50
1:A:430:LEU:HA	1:A:443:LEU:O	2.11	0.50
1:B:430:LEU:CD2	1:B:444:GLU:HB3	2.41	0.50
1:A:211:HIS:CD2	1:A:386:LEU:HD11	2.47	0.50
1:A:253:TRP:CD1	1:A:261:ALA:HB2	2.47	0.50
1:B:375:ILE:HG22	1:B:375:ILE:O	2.12	0.50
1:A:188:TYR:OH	1:A:216:LYS:NZ	2.43	0.49
1:A:221:VAL:HG23	1:A:222:ALA:N	2.27	0.49
1:B:32:LYS:HB2	1:B:405:VAL:HB	1.93	0.49
1:B:34:TYR:C	1:B:34:TYR:CD2	2.90	0.49
1:B:73:LYS:HA	1:B:111:HIS:HD2	1.76	0.49
1:A:77:LYS:HG3	1:A:78:GLU:OE2	2.13	0.49
1:B:224:ILE:HD11	1:B:239:GLY:HA3	1.93	0.49
1:A:418:VAL:HG12	1:B:282:ASP:HA	1.93	0.49
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.46	0.49
1:A:89:GLU:CD	1:B:236:PRO:O	2.55	0.49
1:A:60:TYR:O	1:A:158:PRO:HB2	2.11	0.49
1:A:146:ASN:H	1:A:146:ASN:HD22	1.59	0.49
1:B:103:TYR:HB3	1:B:104:ILE:HD12	1.94	0.49
1:A:374:SER:C	1:A:376:GLU:N	2.70	0.49
1:A:450:LEU:O	1:A:452:GLU:N	2.45	0.49
1:B:409:LEU:HD13	1:B:409:LEU:N	2.28	0.49
1:B:472:SER:C	1:B:474:ASP:N	2.70	0.49
1:B:391:THR:CG2	1:B:393:ASP:HB2	2.42	0.49
1:A:118:ALA:O	1:A:458:LEU:CA	2.58	0.49
1:A:192:ASP:HB2	1:A:386:LEU:CD2	2.43	0.49
1:A:194:GLY:O	1:A:197:GLY:N	2.43	0.49
1:A:156:TRP:CG	1:A:392:ARG:HG3	2.47	0.49
1:A:278:SER:O	1:A:283:ILE:HG13	2.13	0.49
1:B:114:ILE:HD11	1:B:462:PHE:CE2	2.48	0.49
1:A:160:THR:CG2	1:A:394:LEU:HD23	2.43	0.49
1:A:229:LYS:HD3	1:A:230:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TYR:HB3	1:B:375:ILE:HG13	1.95	0.49
1:B:472:SER:OG	1:B:475:GLU:HG3	2.13	0.49
1:A:151:ILE:HG23	1:A:152:LEU:N	2.27	0.48
1:A:211:HIS:CD2	1:A:386:LEU:HD21	2.47	0.48
1:A:342:LYS:HD3	1:A:372:LYS:O	2.13	0.48
1:A:421:PRO:C	1:A:423:LYS:N	2.55	0.48
1:A:430:LEU:HD23	1:A:444:GLU:HA	1.94	0.48
1:B:125:ILE:HG22	1:B:126:PRO:O	2.13	0.48
1:A:229:LYS:O	1:A:229:LYS:HG2	2.12	0.48
1:B:12:LEU:CD2	1:B:80:ILE:HD13	2.43	0.48
1:B:251:THR:HG22	1:B:281:TYR:OH	2.13	0.48
1:A:19:LYS:C	1:A:21:THR:H	2.19	0.48
1:A:247:HIS:HE1	1:A:279:ASP:OD2	1.96	0.48
1:B:167:GLU:O	1:B:168:GLN:C	2.56	0.48
1:B:364:ILE:HG21	1:B:380:PHE:HE2	1.77	0.48
1:B:420:ASP:C	1:B:422:ASN:H	2.22	0.48
1:A:155:SER:C	1:A:157:TYR:H	2.21	0.48
1:A:249:THR:HB	1:B:25:GLN:HB2	1.96	0.48
1:B:158:PRO:HG3	1:B:206:ILE:CG2	2.43	0.48
1:B:263:GLU:HA	1:B:266:VAL:CG2	2.41	0.48
1:A:84:LYS:O	1:A:85:GLU:CB	2.53	0.48
1:A:219:ASP:HA	1:B:17:SER:OG	2.12	0.48
1:A:351:ILE:HA	1:A:379:SER:O	2.13	0.48
1:A:236:PRO:O	1:A:237:VAL:HG23	2.13	0.48
1:A:279:ASP:O	1:A:279:ASP:CG	2.54	0.48
1:A:337:ASN:C	1:A:339:LYS:H	2.21	0.48
1:B:186:LEU:C	1:B:188:TYR:N	2.71	0.48
1:B:388:GLN:O	1:B:389:LYS:HB2	2.13	0.48
1:A:384:GLY:O	1:A:388:GLN:O	2.31	0.48
1:B:136:ASN:HD22	1:B:136:ASN:N	2.11	0.48
1:A:188:TYR:CE2	1:A:216:LYS:HB2	2.49	0.48
1:A:350:VAL:HB	1:A:378:VAL:HG22	1.94	0.48
1:B:430:LEU:HD22	1:B:444:GLU:HB3	1.95	0.48
1:A:196:ARG:NH1	1:B:16:ASP:OD2	2.42	0.48
1:A:472:SER:C	1:A:474:ASP:N	2.71	0.48
1:B:182:ASN:C	1:B:182:ASN:ND2	2.72	0.48
1:B:342:LYS:CG	1:B:372:LYS:O	2.61	0.48
1:A:189:LYS:HZ3	1:A:376:GLU:HA	1.77	0.48
1:B:16:ASP:HB2	1:B:18:TYR:HE2	1.79	0.48
1:B:365:VAL:CG1	1:B:375:ILE:HD12	2.42	0.48
1:B:384:GLY:O	1:B:388:GLN:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LYS:C	1:B:449:ASP:N	2.69	0.48
1:B:153:VAL:C	1:B:155:SER:N	2.64	0.47
1:B:342:LYS:NZ	1:B:373:TRP:CE2	2.82	0.47
1:B:423:LYS:O	1:B:424:ARG:O	2.32	0.47
1:B:482:LEU:CD2	1:B:483:ASN:N	2.76	0.47
1:A:9:PHE:CD2	1:A:10:ASN:N	2.75	0.47
1:A:179:THR:HA	1:A:341:TYR:CE1	2.49	0.47
1:A:208:ALA:HB3	1:A:223:GLY:HA3	1.96	0.47
1:B:9:PHE:CE2	1:B:69:TYR:HD2	2.31	0.47
1:A:283:ILE:CD1	1:A:312:PRO:HA	2.43	0.47
1:B:16:ASP:CB	1:B:18:TYR:HE2	2.26	0.47
1:B:17:SER:O	1:B:20:VAL:HG23	2.14	0.47
1:B:394:LEU:HD12	1:B:394:LEU:N	2.30	0.47
1:B:445:GLU:O	1:B:447:LYS:N	2.47	0.47
1:B:449:ASP:C	1:B:451:GLU:N	2.72	0.47
1:A:250:ILE:HD11	1:A:265:ILE:HD12	1.96	0.47
1:A:263:GLU:HG3	1:A:298:LEU:HD11	1.95	0.47
1:B:71:LYS:CG	1:B:72:GLY:N	2.77	0.47
1:A:56:GLU:HA	1:A:126:PRO:HA	1.96	0.47
1:A:269:PHE:C	1:A:271:SER:N	2.65	0.47
1:A:292:GLY:O	1:A:293:GLU:HG2	2.14	0.47
1:A:299:ILE:C	1:A:301:SER:H	2.23	0.47
1:A:392:ARG:HG2	1:A:397:CYS:HB2	1.96	0.47
1:B:86:VAL:C	1:B:88:ARG:N	2.68	0.47
1:B:374:SER:C	1:B:376:GLU:H	2.23	0.47
1:B:443:LEU:HD11	1:B:453:TYR:CD1	2.49	0.47
1:A:29:ASN:HB3	1:A:407:ASN:OD1	2.15	0.47
1:A:153:VAL:O	1:A:155:SER:N	2.46	0.47
1:A:255:LYS:O	1:A:255:LYS:HD3	2.14	0.47
1:B:446:GLY:O	1:B:449:ASP:HB2	2.14	0.47
1:B:450:LEU:O	1:B:452:GLU:CG	2.59	0.47
1:A:337:ASN:ND2	1:A:339:LYS:HB2	2.29	0.47
1:B:114:ILE:HD11	1:B:462:PHE:HE2	1.79	0.47
1:B:447:LYS:C	1:B:449:ASP:H	2.22	0.47
1:B:102:ASN:HD22	1:B:102:ASN:N	2.13	0.47
1:B:156:TRP:CD1	1:B:392:ARG:HG3	2.49	0.47
1:B:259:LYS:HE3	1:B:294:ASP:HB3	1.97	0.47
1:A:68:LYS:HB2	1:A:230:TYR:CZ	2.50	0.47
1:A:104:ILE:HD12	1:A:113:PRO:HD3	1.96	0.47
1:A:180:SER:HB2	1:A:376:GLU:OE1	2.15	0.47
1:B:275:SER:HB3	2:B:502:IS1:HAT	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:THR:HG22	1:B:392:ARG:N	2.29	0.47
1:A:68:LYS:HE3	1:A:69:TYR:OH	2.15	0.46
1:B:394:LEU:O	1:B:395:LEU:CB	2.63	0.46
1:B:423:LYS:C	1:B:424:ARG:O	2.58	0.46
1:A:13:LEU:O	1:B:221:VAL:CG2	2.63	0.46
1:A:114:ILE:HG13	1:A:114:ILE:O	2.14	0.46
1:B:420:ASP:O	1:B:423:LYS:HB2	2.14	0.46
1:A:86:VAL:O	1:A:88:ARG:N	2.42	0.46
1:A:273:PRO:HG3	1:A:307:PRO:HD2	1.96	0.46
1:B:137:THR:HG21	1:B:464:ASN:OD1	2.16	0.46
1:A:200:SER:HG	1:B:203:THR:HG1	1.58	0.46
1:A:308:LEU:O	1:A:308:LEU:HG	2.13	0.46
1:A:418:VAL:HG11	1:B:282:ASP:OD2	2.16	0.46
1:B:415:LYS:H	1:B:425:SER:CB	2.28	0.46
1:B:455:HIS:CD2	1:B:455:HIS:N	2.84	0.46
1:A:262:PHE:O	1:A:266:VAL:HG22	2.16	0.46
1:B:155:SER:C	1:B:157:TYR:N	2.71	0.46
1:A:35:SER:HA	1:A:401:CYS:HA	1.97	0.46
1:B:327:ILE:O	1:B:331:LYS:HG2	2.15	0.46
1:B:342:LYS:NZ	1:B:373:TRP:CZ2	2.84	0.46
1:B:391:THR:HB	1:B:394:LEU:CD1	2.46	0.46
1:A:248:SER:C	1:A:250:ILE:H	2.23	0.46
1:B:153:VAL:O	1:B:155:SER:N	2.49	0.46
1:A:83:ALA:O	1:A:86:VAL:HB	2.15	0.46
1:A:350:VAL:O	1:A:378:VAL:HA	2.16	0.46
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.71	0.46
1:B:56:GLU:OE2	1:B:124:VAL:HG12	2.15	0.46
1:A:17:SER:OG	1:A:90:HIS:CE1	2.65	0.46
1:A:92:GLN:O	1:A:93:ASP:HB2	2.16	0.46
1:A:289:LYS:HE3	1:A:289:LYS:HB2	1.75	0.46
1:B:311:ARG:NH1	2:B:502:IS1:HAP	2.31	0.46
1:A:151:ILE:CG2	1:A:152:LEU:N	2.78	0.45
1:A:299:ILE:HD12	1:A:308:LEU:HD23	1.99	0.45
1:B:171:ILE:HD12	1:B:171:ILE:N	2.31	0.45
1:A:467:VAL:O	1:A:467:VAL:HG12	2.16	0.45
1:B:18:TYR:CE2	1:B:19:LYS:HD3	2.52	0.45
1:A:427:LYS:HB2	1:A:427:LYS:NZ	2.26	0.45
1:B:155:SER:O	1:B:156:TRP:C	2.60	0.45
1:B:243:PRO:HG3	1:B:269:PHE:CD2	2.51	0.45
1:A:246:GLU:OE1	1:B:19:LYS:NZ	2.42	0.45
1:B:86:VAL:O	1:B:88:ARG:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:NH2	1:B:395:LEU:HA	2.31	0.45
1:B:150:THR:O	1:B:151:ILE:C	2.59	0.45
1:B:304:THR:CG2	1:B:346:PRO:HB3	2.46	0.45
1:A:208:ALA:HB3	1:A:223:GLY:CA	2.46	0.45
1:A:344:LEU:HB3	1:A:345:PRO:HD2	1.98	0.45
1:A:231:TYR:O	1:A:472:SER:HA	2.16	0.45
1:A:243:PRO:CB	1:B:21:THR:HG21	2.46	0.45
1:A:18:TYR:HD1	1:B:244:ALA:HB3	1.81	0.45
1:A:153:VAL:C	1:A:155:SER:N	2.72	0.45
1:A:345:PRO:O	1:A:347:TYR:N	2.49	0.45
1:A:366:GLU:OE1	1:A:370:GLN:OE1	2.35	0.45
1:A:16:ASP:OD2	1:A:150:THR:CG2	2.65	0.45
1:A:33:VAL:HG11	1:A:142:TYR:O	2.17	0.45
1:A:275:SER:HA	1:A:309:ILE:O	2.16	0.45
1:B:10:ASN:C	1:B:10:ASN:OD1	2.59	0.45
1:B:138:ASP:HA	1:B:139:PRO:HD3	1.86	0.45
1:A:26:TYR:C	1:A:27:PRO:O	2.60	0.45
1:B:176:LEU:HD21	1:B:189:LYS:HE3	1.99	0.45
1:B:279:ASP:HB3	1:B:283:ILE:HD12	1.98	0.45
1:A:155:SER:O	1:A:156:TRP:C	2.60	0.45
1:B:62:LEU:O	1:B:66:LEU:CB	2.66	0.45
1:A:119:VAL:HG11	1:A:125:ILE:CD1	2.43	0.44
1:A:239:GLY:C	1:A:240:TYR:CD1	2.96	0.44
1:A:116:VAL:HB	1:A:462:PHE:HB3	1.99	0.44
1:A:299:ILE:O	1:A:302:ARG:HG3	2.16	0.44
1:B:153:VAL:O	1:B:156:TRP:HD1	1.99	0.44
1:B:186:LEU:C	1:B:188:TYR:H	2.23	0.44
1:A:250:ILE:HD13	1:A:261:ALA:HB1	1.98	0.44
1:A:432:LEU:HD13	1:A:457:LEU:HD13	1.99	0.44
1:A:477:ARG:O	1:A:478:LYS:C	2.60	0.44
1:B:157:TYR:O	1:B:158:PRO:C	2.60	0.44
1:A:17:SER:C	1:A:19:LYS:N	2.74	0.44
1:B:211:HIS:CD2	1:B:386:LEU:HD21	2.53	0.44
1:B:432:LEU:HD13	1:B:457:LEU:HD12	1.98	0.44
1:A:244:ALA:HA	1:A:275:SER:O	2.18	0.44
1:A:330:LYS:C	1:A:331:LYS:HD2	2.42	0.44
1:A:414:PHE:CB	1:A:425:SER:HB2	2.47	0.44
1:B:308:LEU:HD21	1:B:310:ILE:CD1	2.45	0.44
1:B:311:ARG:CG	1:B:351:ILE:CG2	2.96	0.44
1:A:13:LEU:O	1:B:221:VAL:HG23	2.18	0.44
1:A:257:HIS:HB3	1:A:260:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:SER:HB3	2:A:501:IS1:HAI	1.98	0.44
1:B:10:ASN:OD1	1:B:11:ILE:N	2.51	0.44
1:B:261:ALA:O	1:B:262:PHE:C	2.61	0.44
1:A:40:ARG:O	1:A:41:GLU:C	2.60	0.44
1:A:102:ASN:O	1:A:103:TYR:C	2.61	0.44
1:A:168:GLN:HG3	1:A:358:ILE:CD1	2.42	0.44
1:A:318:LEU:HD22	1:A:322:LEU:HG	1.99	0.44
1:A:418:VAL:C	1:A:420:ASP:N	2.75	0.44
1:B:16:ASP:HB2	1:B:18:TYR:CE2	2.52	0.44
1:B:135:GLU:O	1:B:135:GLU:HG2	2.17	0.44
1:B:136:ASN:ND2	1:B:136:ASN:O	2.45	0.44
1:B:283:ILE:HD13	1:B:312:PRO:HA	1.97	0.44
1:A:93:ASP:OD2	1:A:95:VAL:CG2	2.66	0.44
2:A:501:IS1:HAXA	2:A:501:IS1:HAM	1.98	0.44
1:A:84:LYS:HE3	1:A:98:GLU:OE1	2.17	0.44
1:A:262:PHE:CD2	1:A:290:ILE:HG21	2.53	0.43
1:A:344:LEU:HB2	1:A:349:ARG:HH12	1.83	0.43
1:B:10:ASN:O	1:B:13:LEU:CD2	2.66	0.43
1:B:192:ASP:OD1	1:B:192:ASP:C	2.61	0.43
1:B:40:ARG:HD3	1:B:400:LYS:NZ	2.33	0.43
1:B:85:GLU:O	1:B:88:ARG:HB3	2.18	0.43
1:B:273:PRO:HG3	1:B:307:PRO:HD2	2.00	0.43
1:B:281:TYR:O	1:B:282:ASP:C	2.61	0.43
1:A:104:ILE:HD12	1:A:113:PRO:CD	2.48	0.43
1:A:134:VAL:HG11	1:A:148:ILE:HD11	1.99	0.43
1:A:157:TYR:HB3	1:A:158:PRO:CD	2.45	0.43
1:A:269:PHE:O	1:A:270:SER:C	2.60	0.43
1:A:314:SER:HB3	1:A:315:GLY:H	1.49	0.43
1:B:16:ASP:CB	1:B:18:TYR:CE2	3.01	0.43
1:A:148:ILE:CD1	1:A:148:ILE:C	2.90	0.43
1:A:273:PRO:HG3	1:A:305:GLU:O	2.17	0.43
1:A:337:ASN:O	1:A:339:LYS:N	2.51	0.43
1:B:13:LEU:H	1:B:13:LEU:CD2	2.21	0.43
1:B:203:THR:HG22	1:B:204:ALA:N	2.32	0.43
1:B:224:ILE:HA	1:B:227:ILE:HD12	1.99	0.43
1:A:10:ASN:OD1	1:A:12:LEU:HB2	2.17	0.43
1:A:291:TRP:CE2	1:A:310:ILE:HD11	2.52	0.43
1:A:387:LEU:HD22	1:A:387:LEU:HA	1.86	0.43
1:B:395:LEU:O	1:B:396:ASN:C	2.61	0.43
1:A:40:ARG:NE	1:A:422:ASN:O	2.51	0.43
1:A:433:HIS:HD2	1:A:443:LEU:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:CG	1:A:10:ASN:N	2.87	0.43
1:A:116:VAL:CG2	1:A:462:PHE:HB3	2.49	0.43
1:A:132:PHE:CD1	1:A:132:PHE:C	2.96	0.43
1:B:309:ILE:HG21	1:B:351:ILE:HB	2.00	0.43
1:B:412:ASN:OD1	1:B:428:GLY:CA	2.66	0.43
1:A:311:ARG:HA	1:A:312:PRO:HD2	1.97	0.43
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.76	0.43
1:A:58:VAL:CG2	1:A:166:ARG:HD3	2.48	0.43
1:A:221:VAL:CG2	1:B:13:LEU:HB2	2.46	0.43
1:B:429:ARG:NH1	1:B:446:GLY:CA	2.79	0.43
1:A:68:LYS:HD3	1:A:69:TYR:CE1	2.54	0.43
1:B:12:LEU:O	1:B:87:TYR:CE1	2.72	0.43
1:B:399:PHE:C	1:B:399:PHE:HD2	2.26	0.43
1:B:406:THR:O	1:B:407:ASN:HB2	2.18	0.43
1:A:296:ARG:O	1:A:299:ILE:HG22	2.19	0.42
1:A:315:GLY:O	1:A:316:ASN:CB	2.67	0.42
1:B:12:LEU:O	1:B:87:TYR:HE1	2.02	0.42
1:B:144:LEU:O	1:B:145:THR:C	2.60	0.42
1:B:380:PHE:CD1	1:B:380:PHE:N	2.87	0.42
1:A:279:ASP:HB3	1:A:283:ILE:HD12	2.00	0.42
1:A:295:LEU:C	1:A:297:HIS:N	2.76	0.42
1:A:328:LEU:HD13	1:A:348:LEU:HD11	2.01	0.42
1:B:56:GLU:OE2	1:B:124:VAL:CG1	2.67	0.42
1:B:447:LYS:HE3	1:B:447:LYS:HB2	1.72	0.42
1:A:221:VAL:CG2	1:B:13:LEU:O	2.68	0.42
1:A:161:VAL:HB	1:A:210:ALA:CB	2.49	0.42
1:A:213:VAL:O	1:A:213:VAL:HG12	2.19	0.42
1:A:297:HIS:C	1:A:299:ILE:N	2.77	0.42
1:B:449:ASP:O	1:B:451:GLU:N	2.50	0.42
1:A:149:GLU:HG3	1:A:399:PHE:CE2	2.53	0.42
1:A:433:HIS:HB2	1:A:441:VAL:HG13	2.01	0.42
1:B:142:TYR:CD1	1:B:142:TYR:C	2.98	0.42
1:A:143:TRP:CD1	1:A:143:TRP:H	2.37	0.42
1:A:203:THR:O	1:A:204:ALA:C	2.62	0.42
1:B:114:ILE:N	1:B:137:THR:CG2	2.83	0.42
1:B:130:VAL:O	1:B:130:VAL:HG13	2.19	0.42
1:A:21:THR:HG21	1:B:243:PRO:CB	2.48	0.42
1:B:394:LEU:O	1:B:395:LEU:HB2	2.19	0.42
1:A:311:ARG:HG3	1:A:351:ILE:CG1	2.46	0.42
1:A:439:THR:HB	1:A:440:PHE:H	1.35	0.42
1:B:36:TYR:HA	1:B:133:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HB2	1:A:107:LYS:HZ2	1.82	0.42
1:A:351:ILE:HG13	1:A:351:ILE:O	2.20	0.42
1:B:136:ASN:ND2	1:B:136:ASN:N	2.67	0.42
1:A:108:TYR:O	1:A:109:ASP:C	2.63	0.41
1:A:158:PRO:HG3	1:A:206:ILE:CG2	2.49	0.41
1:A:206:ILE:CD1	1:A:206:ILE:N	2.82	0.41
1:A:351:ILE:HG22	1:A:379:SER:OG	2.19	0.41
1:B:19:LYS:HA	1:B:22:HIS:CG	2.55	0.41
1:B:413:VAL:HG13	1:B:414:PHE:H	1.82	0.41
1:B:439:THR:HG23	1:B:440:PHE:H	1.79	0.41
1:A:130:VAL:O	1:A:130:VAL:HG13	2.20	0.41
1:A:160:THR:HG22	1:A:390:LEU:HG	2.02	0.41
1:B:289:LYS:HG3	1:B:290:ILE:N	2.35	0.41
1:B:311:ARG:NH1	2:B:502:IS1:CAP	2.83	0.41
1:A:76:THR:O	1:A:77:LYS:C	2.60	0.41
1:A:235:ASP:HB3	1:A:236:PRO:CD	2.50	0.41
1:A:243:PRO:HB3	1:B:21:THR:HG21	2.03	0.41
1:A:263:GLU:HB2	1:A:295:LEU:HD21	2.02	0.41
1:A:283:ILE:O	1:A:283:ILE:CG1	2.68	0.41
1:B:33:VAL:O	1:B:145:THR:HG21	2.20	0.41
1:B:343:LEU:HD12	1:B:377:ASN:OD1	2.20	0.41
1:A:114:ILE:CG2	1:A:144:LEU:HD13	2.50	0.41
1:A:221:VAL:HG21	1:B:13:LEU:CB	2.48	0.41
1:A:418:VAL:CG1	1:A:419:ALA:N	2.83	0.41
1:B:64:TYR:O	1:B:65:ILE:C	2.63	0.41
1:B:337:ASN:ND2	1:B:339:LYS:N	2.53	0.41
1:B:429:ARG:HH11	1:B:446:GLY:HA3	1.81	0.41
1:A:9:PHE:CE2	1:A:11:ILE:HD13	2.56	0.41
1:A:12:LEU:HD22	1:A:101:TRP:CE2	2.54	0.41
1:A:24:LYS:HE2	1:A:24:LYS:HB3	1.83	0.41
1:A:117:LYS:O	1:A:132:PHE:HA	2.19	0.41
1:A:130:VAL:CG1	1:A:130:VAL:O	2.67	0.41
1:A:130:VAL:HG12	1:A:432:LEU:HB2	2.02	0.41
1:A:421:PRO:O	1:A:422:ASN:HB3	2.19	0.41
1:A:11:ILE:O	1:A:11:ILE:HG22	2.19	0.41
1:A:264:HIS:O	1:A:264:HIS:CG	2.73	0.41
1:A:390:LEU:HD12	1:A:390:LEU:HA	1.84	0.41
1:B:155:SER:HA	1:B:158:PRO:HD2	2.03	0.41
1:A:415:LYS:HG2	1:A:425:SER:OG	2.21	0.41
1:B:233:THR:CG2	1:B:235:ASP:HB2	2.51	0.41
1:B:279:ASP:N	1:B:283:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:O	1:A:404:VAL:HG12	2.21	0.41
1:A:88:ARG:C	1:A:88:ARG:HD3	2.46	0.41
1:A:233:THR:HG22	1:A:235:ASP:N	2.36	0.41
1:A:245:ALA:HA	1:B:25:GLN:OE1	2.21	0.41
1:B:147:TRP:C	1:B:147:TRP:CD1	2.99	0.41
1:B:157:TYR:HB3	1:B:158:PRO:CD	2.44	0.41
1:B:212:LEU:HD12	1:B:227:ILE:HD11	2.03	0.41
1:B:250:ILE:HD11	1:B:265:ILE:HD12	2.01	0.41
1:B:313:ASP:O	1:B:314:SER:HB3	2.21	0.41
1:B:388:GLN:O	1:B:389:LYS:CB	2.68	0.41
1:A:18:TYR:CD2	1:B:219:ASP:OD2	2.74	0.41
1:A:202:GLU:O	1:A:206:ILE:CD1	2.58	0.41
1:A:227:ILE:H	1:A:227:ILE:HG13	1.76	0.41
1:B:120:PRO:O	1:B:121:GLU:C	2.63	0.41
1:A:91:PHE:O	1:A:92:GLN:C	2.64	0.40
1:A:120:PRO:HA	1:A:471:TYR:OH	2.21	0.40
1:A:295:LEU:O	1:A:297:HIS:N	2.54	0.40
1:B:54:TYR:OH	1:B:358:ILE:HG21	2.21	0.40
1:A:190:LEU:O	1:A:211:HIS:HE1	2.04	0.40
1:A:221:VAL:CG2	1:A:222:ALA:N	2.83	0.40
1:A:295:LEU:C	1:A:297:HIS:H	2.30	0.40
1:A:423:LYS:O	1:A:424:ARG:C	2.64	0.40
1:A:434:ARG:HE	1:A:434:ARG:HB2	1.75	0.40
1:B:19:LYS:O	1:B:22:HIS:HB2	2.21	0.40
1:B:66:LEU:HD11	1:B:462:PHE:HB2	2.03	0.40
1:B:113:PRO:O	1:B:113:PRO:HG2	2.22	0.40
1:B:412:ASN:HB3	1:B:427:LYS:HB3	2.03	0.40
1:A:360:THR:O	1:A:364:ILE:HG12	2.21	0.40
1:B:32:LYS:O	1:B:404:VAL:HG23	2.21	0.40
1:B:74:VAL:N	1:B:110:GLY:O	2.50	0.40
1:B:151:ILE:CG2	1:B:152:LEU:H	2.33	0.40
1:B:291:TRP:CD1	1:B:310:ILE:HD12	2.57	0.40
1:A:84:LYS:C	1:A:86:VAL:N	2.74	0.40
1:A:87:TYR:HE2	1:B:221:VAL:HG11	1.83	0.40
1:B:10:ASN:ND2	1:B:79:LYS:HB3	2.36	0.40
1:B:55:GLU:HA	1:B:127:ARG:CD	2.52	0.40
1:B:125:ILE:HD12	1:B:125:ILE:N	2.37	0.40
1:B:167:GLU:C	1:B:169:LYS:N	2.79	0.40
1:A:242:VAL:HG13	2:A:501:IS1:HAU	2.03	0.40
1:A:337:ASN:C	1:A:339:LYS:N	2.79	0.40
1:A:477:ARG:HB2	1:A:478:LYS:H	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASP:OD2	1:B:357:ASP:C	2.65	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	459/491 (94%)	372 (81%)	58 (13%)	29 (6%)	1	6
1	B	459/491 (94%)	371 (81%)	61 (13%)	27 (6%)	1	7
All	All	918/982 (94%)	743 (81%)	119 (13%)	56 (6%)	1	7

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	271	SER
1	A	282	ASP
1	B	71	LYS
1	B	72	GLY
1	B	282	ASP
1	B	354	ASP
1	B	414	PHE
1	B	424	ARG
1	B	452	GLU
1	A	154	GLN
1	A	187	GLU
1	A	237	VAL
1	A	338	SER
1	A	346	PRO
1	A	439	THR
1	A	451	GLU

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Mol	Chain	Res	Type
1	A	454	GLY
1	B	22	HIS
1	B	67	ASN
1	B	168	GLN
1	B	187	GLU
1	B	195	TYR
1	B	463	LYS
1	A	17	SER
1	A	126	PRO
1	A	145	THR
1	A	150	THR
1	A	372	LYS
1	A	422	ASN
1	A	478	LYS
1	B	154	GLN
1	B	236	PRO
1	B	288	GLU
1	B	375	ILE
1	A	232	GLY
1	A	316	ASN
1	A	456	ASP
1	A	477	ARG
1	B	113	PRO
1	B	338	SER
1	B	469	LYS
1	A	71	LYS
1	A	93	ASP
1	A	421	PRO
1	B	167	GLU
1	B	283	ILE
1	B	410	GLY
1	A	296	ARG
1	B	372	LYS
1	A	194	GLY
1	A	283	ILE
1	B	139	PRO
1	B	418	VAL
1	B	446	GLY
1	A	157	TYR

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	408/431 (95%)	336 (82%)	72 (18%)	2	10
1	B	408/431 (95%)	338 (83%)	70 (17%)	2	11
All	All	816/862 (95%)	674 (83%)	142 (17%)	2	10

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	13	LEU
1	A	19	LYS
1	A	24	LYS
1	A	30	THR
1	A	32	LYS
1	A	33	VAL
1	A	34	TYR
1	A	77	LYS
1	A	88	ARG
1	A	89	GLU
1	A	107	LYS
1	A	119	VAL
1	A	144	LEU
1	A	150	THR
1	A	151	ILE
1	A	174	LYS
1	A	179	THR
1	A	180	SER
1	A	186	LEU
1	A	187	GLU
1	A	189	LYS
1	A	190	LEU
1	A	192	ASP
1	A	195	TYR
1	A	196	ARG
1	A	206	ILE

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Mol	Chain	Res	Type
1	A	216	LYS
1	A	219	ASP
1	A	224	ILE
1	A	228	LYS
1	A	234	LYS
1	A	237	VAL
1	A	275	SER
1	A	294	ASP
1	A	295	LEU
1	A	305	GLU
1	A	316	ASN
1	A	318	LEU
1	A	324	VAL
1	A	331	LYS
1	A	334	VAL
1	A	335	SER
1	A	342	LYS
1	A	349	ARG
1	A	352	GLN
1	A	354	ASP
1	A	366	GLU
1	A	368	MET
1	A	369	LYS
1	A	371	LYS
1	A	374	SER
1	A	376	GLU
1	A	379	SER
1	A	387	LEU
1	A	390	LEU
1	A	391	THR
1	A	398	SER
1	A	404	VAL
1	A	409	LEU
1	A	414	PHE
1	A	424	ARG
1	A	431	SER
1	A	432	LEU
1	A	439	THR
1	A	441	VAL
1	A	451	GLU
1	A	452	GLU
1	A	457	LEU

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Mol	Chain	Res	Type
1	A	458	LEU
1	A	482	LEU
1	A	483	ASN
1	B	11	ILE
1	B	13	LEU
1	B	18	TYR
1	B	19	LYS
1	B	34	TYR
1	B	66	LEU
1	B	70	LEU
1	B	76	THR
1	B	85	GLU
1	B	92	GLN
1	B	94	ASP
1	B	99	ARG
1	B	102	ASN
1	B	107	LYS
1	B	119	VAL
1	B	136	ASN
1	B	137	THR
1	B	138	ASP
1	B	144	LEU
1	B	150	THR
1	B	165	SER
1	B	180	SER
1	B	182	ASN
1	B	186	LEU
1	B	190	LEU
1	B	195	TYR
1	B	203	THR
1	B	219	ASP
1	B	224	ILE
1	B	226	LEU
1	B	233	THR
1	B	235	ASP
1	B	237	VAL
1	B	242	VAL
1	B	258	GLU
1	B	275	SER
1	B	277	VAL
1	B	334	VAL
1	B	337	ASN

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Mol	Chain	Res	Type
1	B	338	SER
1	B	342	LYS
1	B	344	LEU
1	B	351	ILE
1	B	352	GLN
1	B	354	ASP
1	B	360	THR
1	B	368	MET
1	B	376	GLU
1	B	386	LEU
1	B	387	LEU
1	B	389	LYS
1	B	390	LEU
1	B	394	LEU
1	B	395	LEU
1	B	399	PHE
1	B	406	THR
1	B	409	LEU
1	B	423	LYS
1	B	429	ARG
1	B	431	SER
1	B	432	LEU
1	B	444	GLU
1	B	445	GLU
1	B	451	GLU
1	B	452	GLU
1	B	455	HIS
1	B	460	THR
1	B	463	LYS
1	B	481	GLN
1	B	482	LEU

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

Mol	Chain	Res	Type
1	A	22	HIS
1	A	67	ASN
1	A	81	GLN
1	A	90	HIS
1	A	92	GLN
1	A	102	ASN
1	A	111	HIS

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Mol	Chain	Res	Type
1	A	129	ASN
1	A	146	ASN
1	A	164	ASN
1	A	182	ASN
1	A	211	HIS
1	A	316	ASN
1	A	388	GLN
1	A	396	ASN
1	A	433	HIS
1	B	22	HIS
1	B	81	GLN
1	B	90	HIS
1	B	102	ASN
1	B	111	HIS
1	B	129	ASN
1	B	136	ASN
1	B	146	ASN
1	B	164	ASN
1	B	168	GLN
1	B	182	ASN
1	B	201	GLN
1	B	211	HIS
1	B	214	ASN
1	B	257	HIS
1	B	337	ASN
1	B	370	GLN
1	B	396	ASN
1	B	422	ASN
1	B	455	HIS
1	B	459	HIS
1	B	481	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are 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	IS1	A	501	-	39,41,41	1.61	7 (17%)	50,55,55	2.25	10 (20%)
2	IS1	B	502	-	39,41,41	1.53	8 (20%)	50,55,55	1.90	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IS1	A	501	-	-	2/27/53/53	0/4/4/4
2	IS1	B	502	-	-	6/27/53/53	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IS1	O4'-C4'	-5.18	1.33	1.45
2	B	502	IS1	CAP-NBL	4.87	1.40	1.35
2	B	502	IS1	CAF-CBB	-4.52	1.38	1.48
2	A	501	IS1	CAP-NBL	4.42	1.39	1.35
2	A	501	IS1	CAF-CBB	-4.10	1.39	1.48
2	B	502	IS1	CBD-CAG	-2.97	1.39	1.47
2	B	502	IS1	O4'-C1'	2.87	1.44	1.40
2	A	501	IS1	CBD-CAG	-2.80	1.39	1.47
2	B	502	IS1	CAF-CAG	2.64	1.39	1.33
2	A	501	IS1	O4'-C1'	2.36	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	IS1	O5'-C5'	2.33	1.52	1.42
2	A	501	IS1	CAF-CAG	2.25	1.38	1.33
2	B	502	IS1	CAO-NBL	2.17	1.40	1.35
2	A	501	IS1	CBE-CBC	2.09	1.53	1.50
2	B	502	IS1	CBE-CBC	2.08	1.53	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IS1	O3'-C3'-C2'	7.54	135.98	111.82
2	B	502	IS1	O3'-C3'-C4'	7.32	132.12	111.08
2	B	502	IS1	O4'-C4'-C5'	6.61	123.19	109.22
2	A	501	IS1	C5'-C4'-C3'	6.18	129.68	115.10
2	A	501	IS1	CAX-NBK-CAY	5.05	122.97	112.68
2	A	501	IS1	C2'-C3'-C4'	-5.03	92.90	102.61
2	A	501	IS1	O3'-C3'-C4'	4.80	124.86	111.08
2	A	501	IS1	C4'-O4'-C1'	-4.37	105.92	109.92
2	B	502	IS1	CAX-NBK-CAY	4.20	121.25	112.68
2	B	502	IS1	C4'-O4'-C1'	-4.12	106.16	109.92
2	A	501	IS1	CBD-CAG-CAF	-3.99	118.21	126.92
2	A	501	IS1	CBD-CAP-NBL	-2.99	118.74	121.28
2	B	502	IS1	CBD-CAG-CAF	-2.89	120.60	126.92
2	A	501	IS1	CAR-CAT-NAZ	-2.31	105.72	112.20
2	B	502	IS1	CAR-CAT-NAZ	-2.12	106.24	112.20
2	A	501	IS1	CAS-CAU-CBF	-2.06	103.41	115.76
2	B	502	IS1	CAO-NBL-CAP	-2.05	120.13	121.88

There are no chirality outliers.

All (8) torsion outliers are listed below:

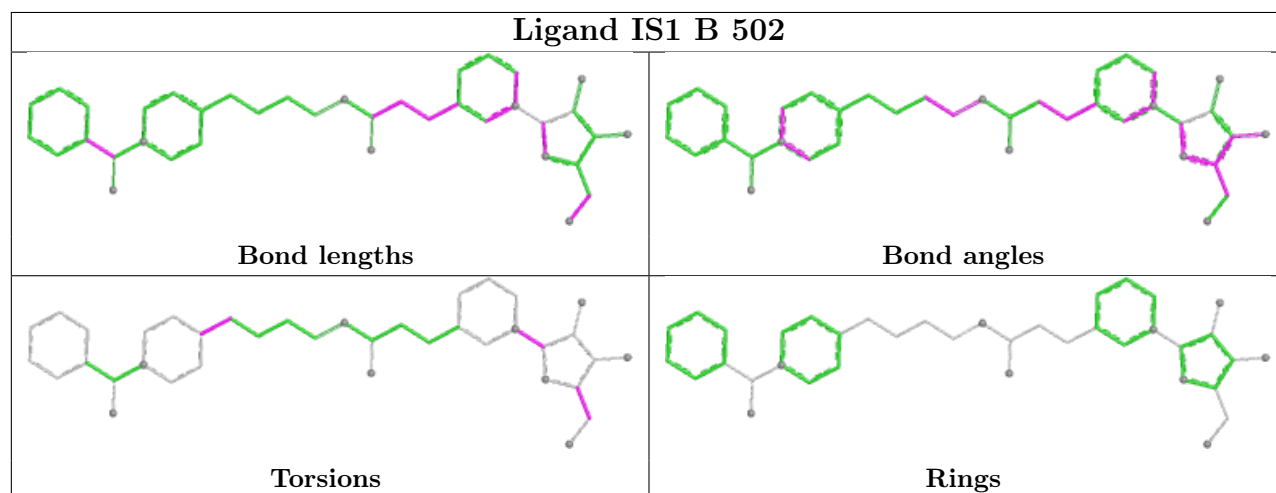
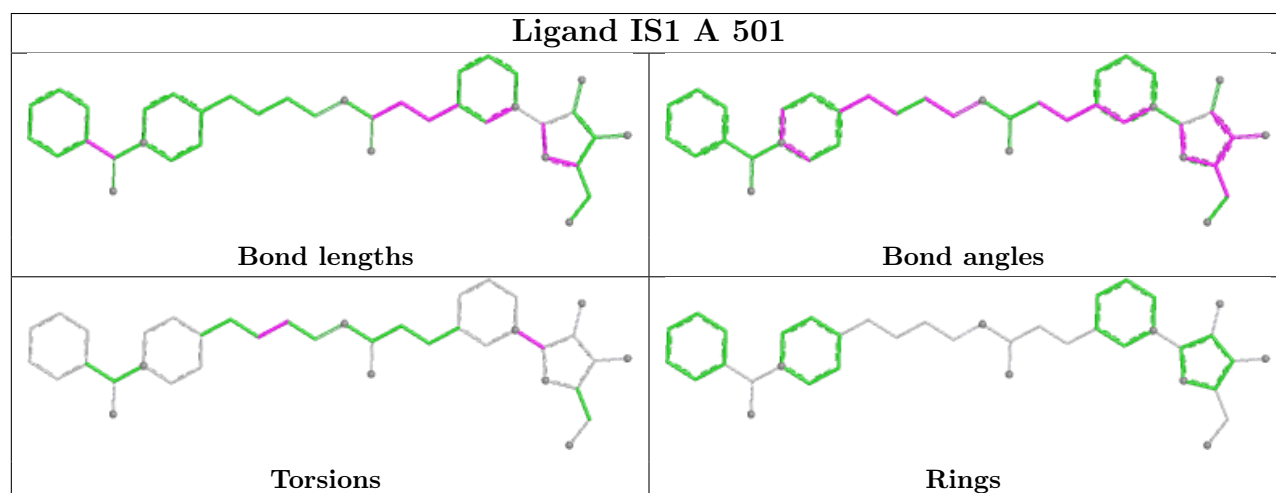
Mol	Chain	Res	Type	Atoms
2	A	501	IS1	C2'-C1'-NBL-CAP
2	B	502	IS1	C2'-C1'-NBL-CAO
2	B	502	IS1	C3'-C4'-C5'-O5'
2	A	501	IS1	CAT-CAR-CAS-CAU
2	B	502	IS1	CAS-CAU-CBF-CAW
2	B	502	IS1	CAS-CAU-CBF-CAV
2	B	502	IS1	C2'-C1'-NBL-CAP
2	B	502	IS1	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IS1	15	0
2	B	502	IS1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	463/491 (94%)	0.19	7 (1%) 72 49	7, 33, 56, 78	0
1	B	463/491 (94%)	0.11	4 (0%) 81 61	10, 32, 55, 79	0
All	All	926/982 (94%)	0.15	11 (1%) 76 55	7, 33, 56, 79	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ASN	4.2
1	A	235	ASP	3.1
1	A	237	VAL	2.9
1	B	237	VAL	2.8
1	A	9	PHE	2.2
1	A	455	HIS	2.2
1	B	394	LEU	2.1
1	A	233	THR	2.1
1	B	30	THR	2.1
1	A	240	TYR	2.1
1	B	136	ASN	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](#)

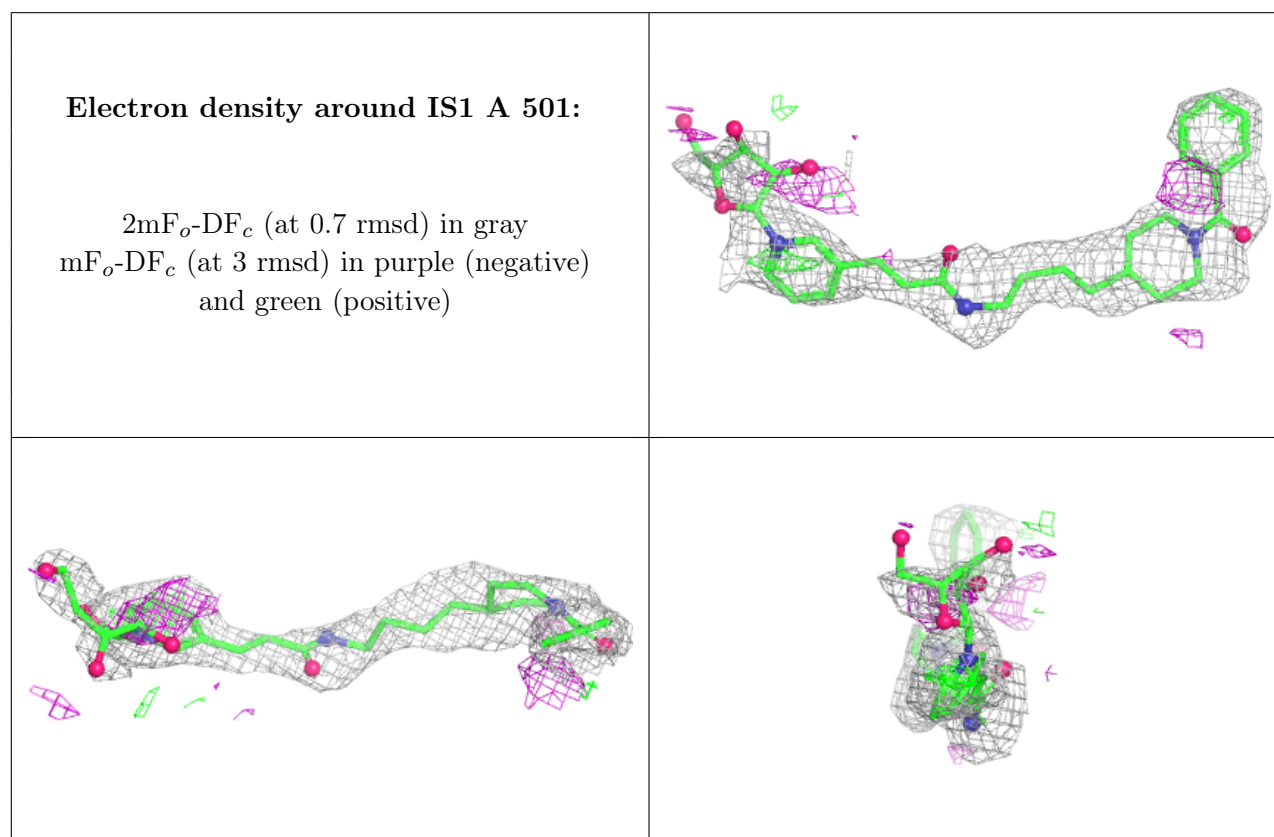
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

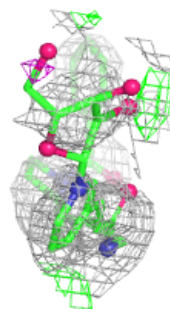
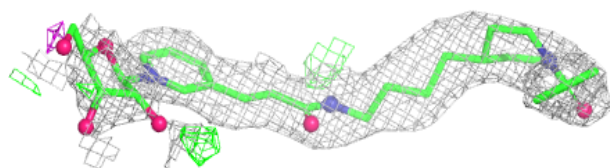
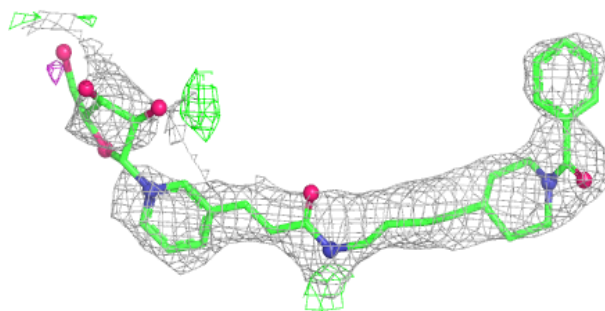
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IS1	A	501	38/38	0.74	0.22	54,64,87,89	0
2	IS1	B	502	38/38	0.77	0.20	56,62,78,83	0

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.



Electron density around IS1 B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.