



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:40 AM EDT

PDB ID : 2AJL / pdb_00002ajl
Title : X-ray Structure of Novel Biaryl-Based Dipeptidyl peptidase IV inhibitor
Authors : Qiao, L.; Baumann, C.A.; Crysler, C.S.; Ninan, N.S.; Abad, M.C.; Spurlino, J.C.; DesJarlais, R.L.; Kervinen, J.; Neeper, M.P.; Bayoumy, S.S.
Deposited on : 2005-08-02
Resolution : 2.50 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

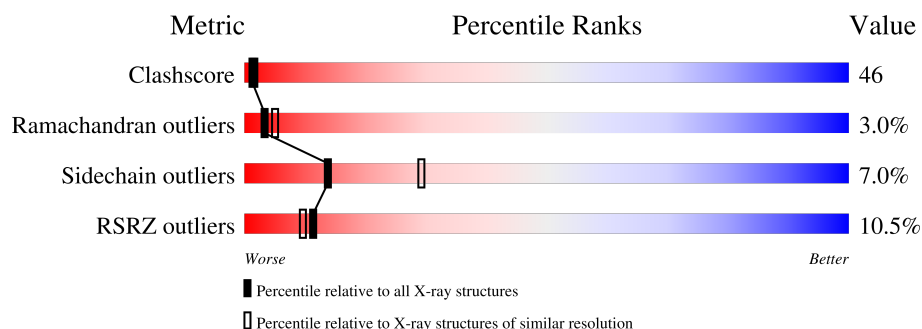
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	I	728	
1	J	728	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	I	768	X	-	-	-
2	NAG	I	771	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	J	767	-	-	X	-
2	NAG	J	769	X	-	-	-
2	NAG	J	771	X	-	-	-
3	JNH	J	1	X	-	-	-

2 Entry composition [i](#)

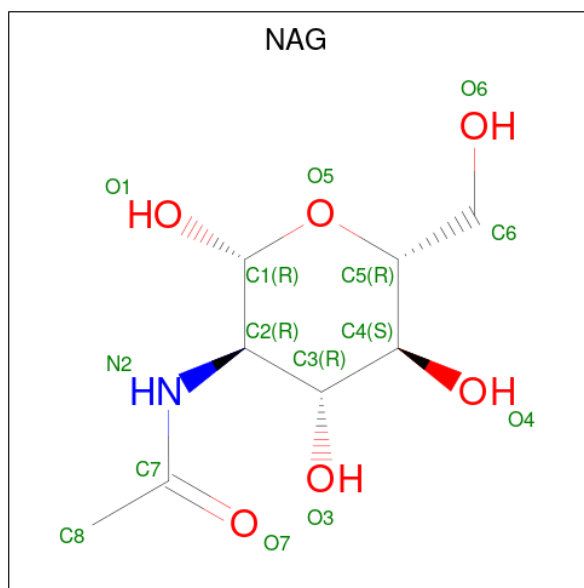
There are 4 unique types of molecules in this entry. The entry contains 12558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	726	Total	C	N	O	S	0	0	0
			5947	3818	977	1126	26			
1	J	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



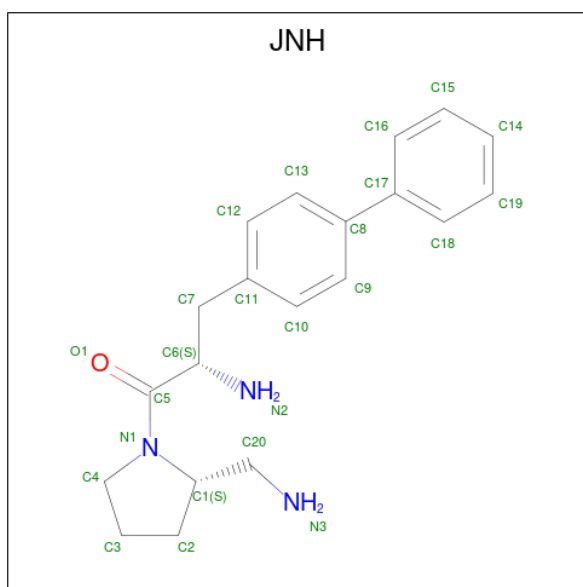
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 1-[2-(S)-AMINO-3-BIPHENYL-4-YL-PROPIONYL]-PYRROLIDINE-2-(S)-CARBONITRILE (CCD ID: JNH) (formula: $C_{20}H_{25}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			24	20	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	0	0
			24	20	3	1		

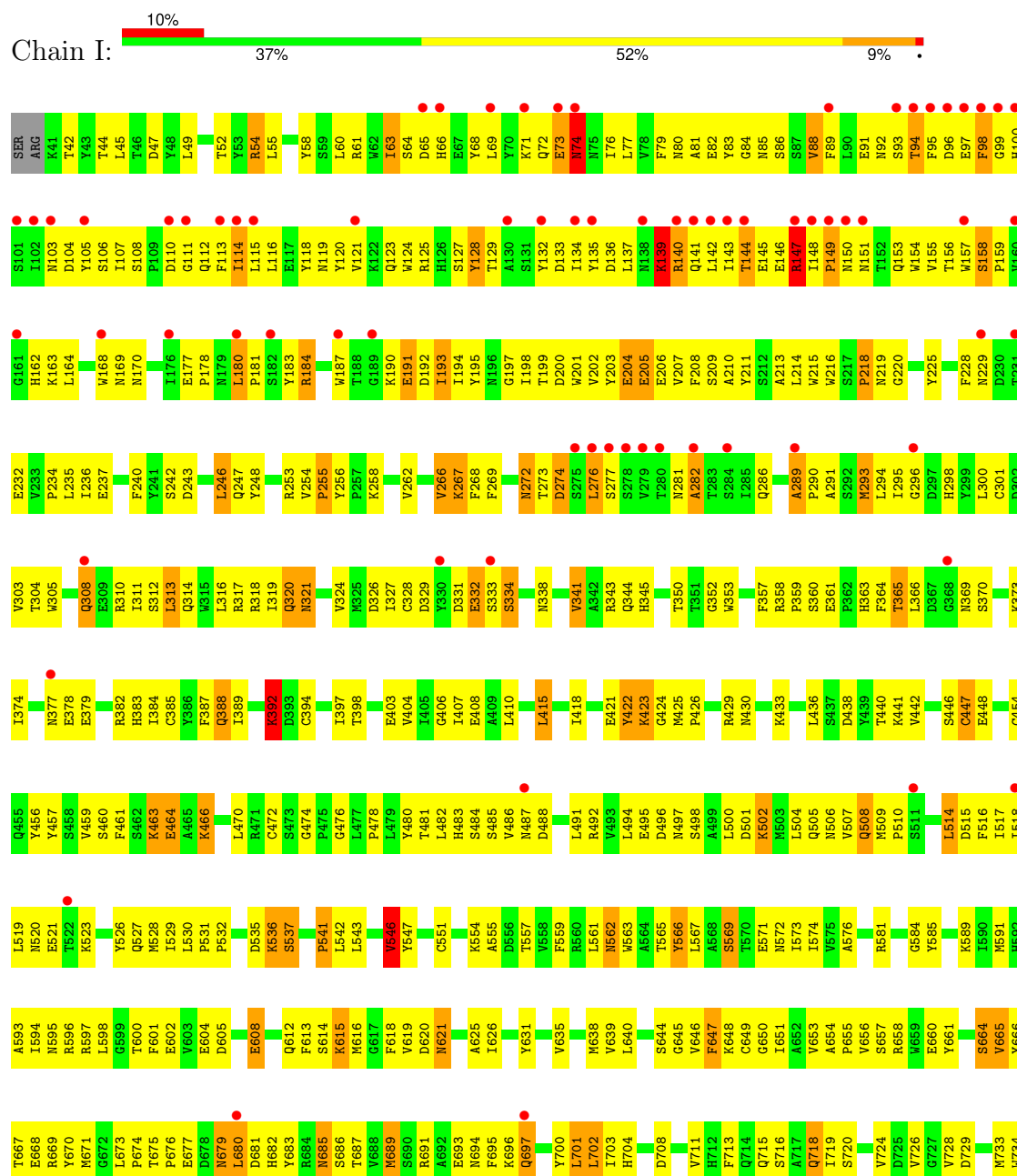
- Molecule 4 is water.

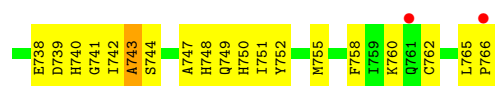
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	190	Total	O	0	0
			190	190		
4	J	213	Total	O	0	0
			213	213		

3 Residue-property plots

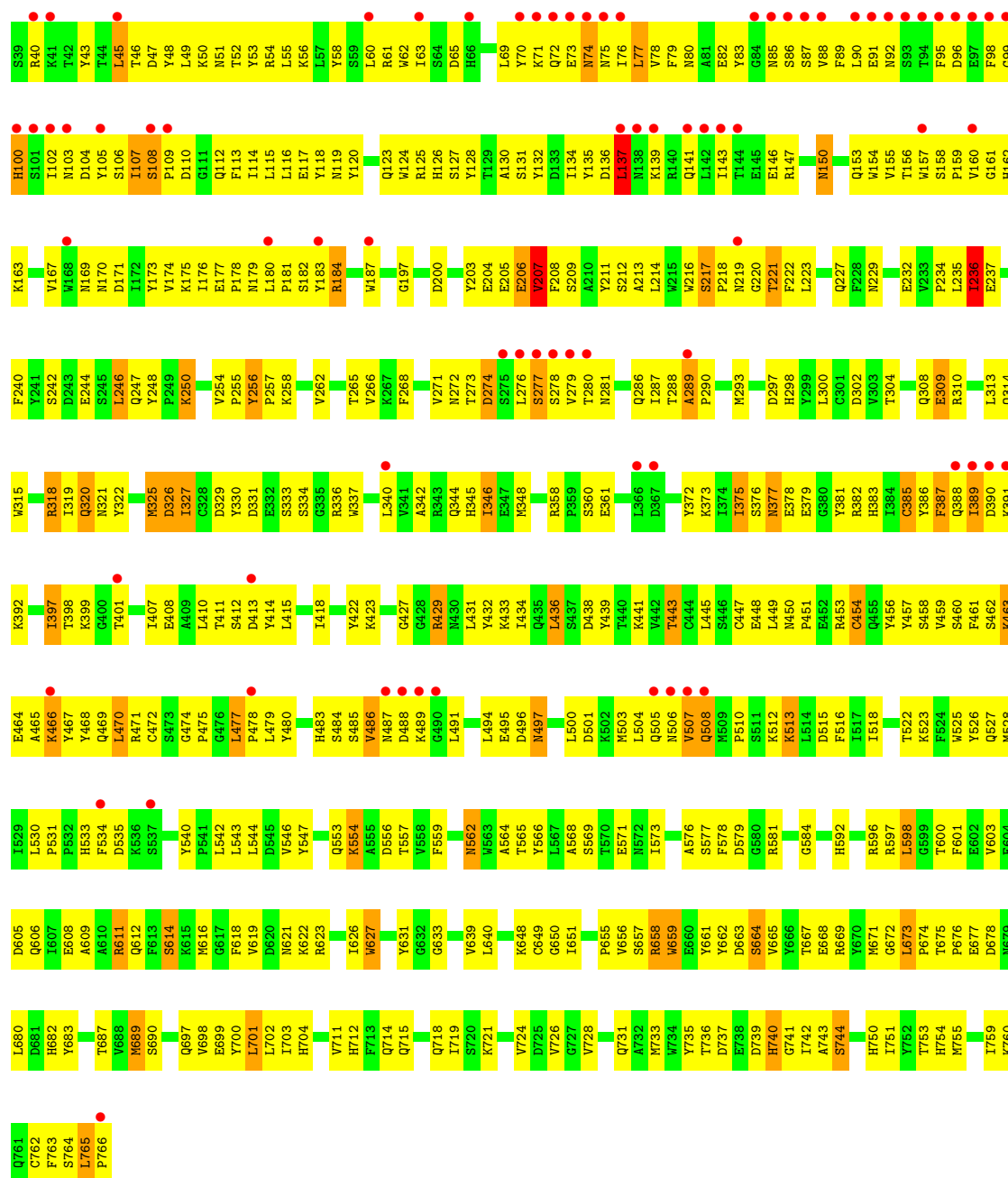
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 4





● Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.28Å 126.88Å 110.83Å 90.00° 99.41° 90.00°	Depositor
Resolution (Å)	64.10 – 2.50 64.10 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.8 (64.10-2.50) 91.6 (64.10-2.51)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.303 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12558	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: NAG, JNH

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	I	0.43	0/6119	0.99	37/8322 (0.4%)
1	J	0.44	0/6136	1.01	28/8344 (0.3%)
All	All	0.44	0/12255	1.00	65/16666 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	378	GLU	N-CA-C	-10.03	100.45	112.89
1	I	300	LEU	N-CA-C	-8.40	95.55	109.24
1	I	388	GLN	N-CA-C	-8.37	94.77	108.41
1	I	656	VAL	N-CA-C	-7.60	97.11	109.12
1	J	206	GLU	N-CA-C	7.54	122.55	113.12
1	I	766	PRO	CA-C-O	7.39	143.17	121.00
1	J	63	ILE	N-CA-C	-7.28	105.49	113.43
1	I	205	GLU	N-CA-C	7.25	119.27	111.36
1	J	300	LEU	N-CA-C	-7.17	97.04	108.73
1	J	766	PRO	CA-C-O	7.09	142.28	121.00
1	I	448	GLU	N-CA-C	6.96	121.78	113.28
1	J	240	PHE	N-CA-C	-6.92	96.78	108.26
1	I	319	ILE	N-CA-C	-6.84	97.65	107.37
1	J	466	LYS	N-CA-C	-6.82	103.64	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	659	TRP	N-CA-C	6.77	120.64	112.38
1	J	397	ILE	N-CA-C	-6.75	106.14	112.83
1	I	266	VAL	N-CA-C	6.74	118.06	108.42
1	I	364	PHE	N-CA-C	6.74	120.00	110.50
1	I	236	ILE	N-CA-C	-6.73	98.64	108.87
1	I	546	VAL	N-CA-C	6.68	119.99	108.90
1	J	200	ASP	N-CA-C	-6.51	100.82	110.46
1	J	274	ASP	N-CA-C	-6.43	105.08	113.12
1	J	150	ASN	N-CA-C	-6.42	101.02	110.52
1	J	319	ILE	N-CA-C	-6.39	97.28	106.55
1	J	108	SER	CA-C-N	6.37	126.85	119.47
1	J	108	SER	C-N-CA	6.37	126.85	119.47
1	I	392	LYS	N-CA-C	6.00	118.58	111.33
1	I	158	SER	N-CA-C	-5.90	101.54	110.39
1	I	743	ALA	N-CA-C	5.89	120.62	113.38
1	I	686	SER	N-CA-C	5.88	119.42	112.72
1	J	412	SER	N-CA-C	-5.85	105.40	112.54
1	I	240	PHE	N-CA-C	-5.85	98.75	108.34
1	J	454	CYS	N-CA-C	5.82	117.87	107.80
1	I	569	SER	N-CA-C	5.73	118.47	111.82
1	J	458	SER	N-CA-C	-5.71	100.38	109.23
1	I	700	TYR	N-CA-C	5.67	118.72	109.59
1	J	483	HIS	N-CA-C	5.67	117.59	109.14
1	J	236	ILE	N-CA-C	-5.60	100.35	108.36
1	I	139	LYS	N-CA-C	-5.60	105.80	113.30
1	I	180	LEU	CA-C-N	5.58	125.58	119.89
1	I	180	LEU	C-N-CA	5.58	125.58	119.89
1	I	254	VAL	N-CA-C	5.57	114.23	107.61
1	J	584	GLY	N-CA-C	5.52	121.31	112.58
1	I	466	LYS	N-CA-C	-5.51	105.68	112.90
1	I	63	ILE	N-CA-C	-5.50	106.99	113.42
1	I	485	SER	N-CA-C	5.50	117.27	111.28
1	J	614	SER	N-CA-C	-5.47	106.45	113.01
1	I	647	PHE	N-CA-C	5.45	118.70	109.76
1	I	529	ILE	N-CA-C	-5.40	99.31	107.73
1	J	664	SER	N-CA-C	5.39	117.60	111.02
1	J	753	THR	N-CA-C	-5.32	105.38	111.07
1	I	320	GLN	N-CA-C	5.29	122.08	110.80
1	J	217	SER	N-CA-C	-5.28	103.38	109.93
1	J	470	LEU	N-CA-C	-5.24	101.99	110.32
1	I	667	THR	N-CA-C	5.23	116.83	111.03
1	I	365	THR	N-CA-C	-5.17	103.71	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	207	VAL	N-CA-C	5.13	116.55	111.67
1	I	201	TRP	N-CA-C	5.11	116.54	110.97
1	I	74	ASN	N-CA-C	-5.07	106.84	112.57
1	I	562	ASN	N-CA-C	5.06	115.05	108.07
1	I	255	PRO	N-CA-C	-5.05	102.06	112.47
1	J	744	SER	N-CA-C	-5.02	103.85	110.33
1	J	137	LEU	N-CA-C	-5.02	106.67	112.89
1	I	541	PRO	N-CA-C	-5.01	103.42	111.38
1	I	537	SER	N-CA-C	-5.00	106.03	112.68

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	700	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	5947	0	5666	559	0
1	J	5964	0	5684	532	0
2	I	70	0	65	8	0
2	J	126	0	117	22	0
3	I	24	0	24	8	0
3	J	24	0	23	7	0
4	I	190	0	0	19	0
4	J	213	0	0	13	0
All	All	12558	0	11579	1087	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 46.

All (1087) 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:J:489:LYS:HE3	1:J:491:LEU:HD21	1.27	1.14
1:I:289:ALA:HB1	1:I:290:PRO:HA	1.28	1.13
1:I:107:ILE:HG13	1:I:114:ILE:HG12	1.23	1.11
1:J:293:MET:HE3	1:J:315:TRP:HB2	1.25	1.10
1:I:310:ARG:HD3	1:I:329:ASP:OD1	1.51	1.10
1:I:626:ILE:HD13	1:I:639:VAL:HG21	1.34	1.10
1:J:40:ARG:HB2	1:J:508:GLN:HE22	1.17	1.09
1:J:389:ILE:HG13	1:J:390:ASP:H	1.15	1.09
1:I:74:ASN:HD22	1:I:92:ASN:ND2	1.54	1.06
1:I:74:ASN:HB2	1:I:92:ASN:HB3	1.39	1.04
1:I:289:ALA:HB1	1:I:290:PRO:CA	1.89	1.02
1:I:392:LYS:HE3	1:I:392:LYS:HA	1.38	1.02
1:I:528:MET:HE2	1:I:530:LEU:HD21	1.40	1.01
1:J:78:VAL:HG13	1:J:89:PHE:HB2	1.39	1.01
1:J:289:ALA:HB1	1:J:290:PRO:HA	1.40	1.01
1:I:594:ILE:HD13	1:I:598:LEU:HD23	1.42	1.01
1:J:106:SER:HB3	1:J:115:LEU:HB3	1.45	0.99
1:J:383:HIS:ND1	1:J:398:THR:HG22	1.77	0.98
1:J:289:ALA:HB1	1:J:290:PRO:CA	1.93	0.97
1:J:65:ASP:HA	1:J:462:SER:HB2	1.41	0.96
1:I:751:ILE:HG12	1:I:755:MET:HE2	1.45	0.95
1:I:671:MET:HE1	1:I:682:HIS:HD2	1.30	0.95
1:J:516:PHE:CE2	1:J:523:LYS:HE3	2.01	0.95
1:J:136:ASP:HB3	1:J:139:LYS:HG2	1.49	0.94
1:I:237:GLU:OE2	1:I:253:ARG:HD2	1.66	0.94
1:I:640:LEU:HD11	1:I:650:GLY:HA3	1.48	0.94
1:J:219:ASN:HD22	1:J:221:THR:CG2	1.80	0.93
1:I:422:TYR:CE2	1:I:423:LYS:HD3	2.04	0.93
1:J:229:ASN:HD21	2:J:771:NAG:C1	1.81	0.93
1:J:293:MET:HE3	1:J:315:TRP:CB	1.98	0.93
1:I:410:LEU:HD13	1:I:415:LEU:HD23	1.50	0.92
1:J:689:MET:HE1	1:J:718:GLN:C	1.94	0.92
1:I:107:ILE:HD12	1:I:114:ILE:HG23	1.52	0.92
1:I:671:MET:HE1	1:I:682:HIS:CD2	2.04	0.91
1:I:528:MET:HE3	1:I:574:ILE:HG21	1.51	0.91
1:I:314:GLN:HE22	1:I:373:LYS:NZ	1.69	0.91
1:I:631:TYR:HB2	3:I:1:JNH:H22	1.52	0.91
1:J:389:ILE:HG13	1:J:390:ASP:N	1.84	0.91
1:I:502:LYS:O	1:I:505:GLN:HG2	1.71	0.91
1:I:631:TYR:H	3:I:1:JNH:H201	1.37	0.89
1:J:489:LYS:HE3	1:J:491:LEU:CD2	2.03	0.89
1:I:42:THR:HG22	1:I:508:GLN:HB2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:571:GLU:CD	1:I:760:LYS:HD3	1.98	0.89
1:J:114:ILE:HG22	1:J:137:LEU:HD21	1.55	0.89
1:I:74:ASN:O	1:I:92:ASN:HB3	1.73	0.89
1:I:267:LYS:HB3	1:I:269:PHE:CE1	2.08	0.89
1:J:40:ARG:CB	1:J:508:GLN:HE22	1.85	0.88
1:J:611:ARG:HG3	1:J:611:ARG:HH11	1.37	0.88
1:J:318:ARG:HH12	1:J:664:SER:HB2	1.39	0.86
1:I:500:LEU:HG	1:I:504:LEU:HD12	1.57	0.86
1:I:626:ILE:CD1	1:I:639:VAL:HG21	2.06	0.86
1:J:526:TYR:HE2	1:J:528:MET:HE3	1.41	0.86
1:I:74:ASN:HD22	1:I:92:ASN:HD22	1.16	0.85
1:J:85:ASN:HD21	2:J:767:NAG:C1	1.90	0.85
1:I:594:ILE:HD13	1:I:598:LEU:CD2	2.05	0.85
1:J:77:LEU:N	1:J:77:LEU:HD23	1.91	0.85
1:I:463:LYS:O	1:I:464:GLU:HG3	1.76	0.85
1:I:648:LYS:HE3	1:I:762:CYS:O	1.77	0.85
1:J:114:ILE:HG23	1:J:135:TYR:HB3	1.59	0.85
1:I:193:ILE:HG22	1:I:194:ILE:HG12	1.58	0.84
1:J:293:MET:CE	1:J:315:TRP:HB2	2.07	0.84
1:I:96:ASP:CG	1:I:97:GLU:H	1.85	0.84
1:J:614:SER:HA	1:J:619:VAL:HB	1.59	0.84
1:I:118:TYR:O	1:I:119:ASN:HB2	1.76	0.84
1:J:219:ASN:HD22	1:J:221:THR:HG23	1.43	0.84
1:I:107:ILE:HG13	1:I:114:ILE:CG1	2.05	0.83
1:J:114:ILE:CG2	1:J:135:TYR:HB3	2.09	0.83
1:J:74:ASN:O	1:J:92:ASN:HB2	1.76	0.83
1:I:146:GLU:OE1	1:I:181:PRO:HG3	1.79	0.83
1:J:258:LYS:HZ1	1:J:712:HIS:HD2	1.25	0.83
1:J:571:GLU:OE2	1:J:760:LYS:HD3	1.79	0.82
1:I:115:LEU:HD11	1:I:132:TYR:HB3	1.60	0.82
1:I:184:ARG:NH1	1:I:187:TRP:HA	1.95	0.81
1:I:74:ASN:HB2	1:I:92:ASN:CB	2.09	0.81
1:J:40:ARG:HB2	1:J:508:GLN:NE2	1.93	0.81
1:J:500:LEU:HA	1:J:503:MET:CE	2.09	0.81
1:J:377:ASN:C	1:J:377:ASN:HD22	1.85	0.81
1:J:258:LYS:NZ	1:J:712:HIS:HD2	1.78	0.81
1:J:82:GLU:HG2	1:J:83:TYR:CE1	2.16	0.80
1:I:74:ASN:ND2	1:I:92:ASN:ND2	2.30	0.79
1:I:363:HIS:CE1	1:I:407:ILE:HB	2.17	0.79
1:I:72:GLN:HB3	1:I:77:LEU:HD13	1.64	0.79
1:I:674:PRO:O	1:I:680:LEU:HB2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:ASP:CB	1:J:139:LYS:HG2	2.13	0.78
1:I:202:VAL:HG12	4:I:788:HOH:O	1.83	0.78
1:J:487:ASN:ND2	1:J:489:LYS:HB3	1.99	0.78
1:J:500:LEU:HA	1:J:503:MET:HE3	1.66	0.78
1:I:74:ASN:ND2	1:I:92:ASN:HD22	1.80	0.78
1:I:369:ASN:O	1:I:389:ILE:HG12	1.84	0.78
1:J:289:ALA:CB	1:J:290:PRO:HA	2.14	0.78
1:J:219:ASN:HB2	1:J:308:GLN:OE1	1.84	0.77
1:I:242:SER:HB3	1:I:246:LEU:HD12	1.65	0.77
1:I:408:GLU:HG3	1:I:459:VAL:CG1	2.15	0.77
1:J:88:VAL:HG11	1:J:91:GLU:HG2	1.64	0.77
1:I:272:ASN:C	1:I:272:ASN:HD22	1.91	0.77
1:J:314:GLN:CG	1:J:325:MET:HG2	2.15	0.77
1:I:289:ALA:CB	1:I:290:PRO:HA	2.13	0.77
1:I:290:PRO:HG3	1:I:326:ASP:OD2	1.84	0.77
1:J:118:TYR:CE2	1:J:119:ASN:ND2	2.53	0.77
1:I:267:LYS:HB3	1:I:269:PHE:HE1	1.47	0.77
1:I:89:PHE:HE1	1:I:114:ILE:HD11	1.49	0.77
1:J:45:LEU:HD22	1:J:49:LEU:HG	1.67	0.77
1:J:633:GLY:HA3	1:J:655:PRO:HB3	1.67	0.76
1:I:159:PRO:HD3	1:I:216:TRP:HB3	1.66	0.76
1:J:203:TYR:HA	1:J:207:VAL:HG13	1.67	0.76
1:I:528:MET:HE2	1:I:530:LEU:CD2	2.14	0.76
1:J:114:ILE:CG2	1:J:137:LEU:HD21	2.15	0.76
1:J:229:ASN:HD21	2:J:771:NAG:C2	1.97	0.76
1:J:518:ILE:CD1	1:J:523:LYS:HB3	2.15	0.76
1:I:98:PHE:O	1:I:100:HIS:N	2.18	0.75
1:J:236:ILE:HG13	1:J:712:HIS:NE2	2.01	0.75
1:J:321:ASN:HD21	2:J:774:NAG:C7	2.00	0.75
1:J:77:LEU:HD23	1:J:77:LEU:H	1.48	0.75
1:J:217:SER:HB3	1:J:222:PHE:HB2	1.68	0.75
1:J:322:TYR:CD1	1:J:348:MET:HE3	2.21	0.75
1:J:60:LEU:HD13	1:J:469:GLN:OE1	1.87	0.74
1:J:598:LEU:HB2	1:J:671:MET:SD	2.27	0.74
1:J:286:GLN:HE21	1:J:288:THR:HG22	1.51	0.74
1:I:459:VAL:HG21	1:I:461:PHE:CE1	2.21	0.74
1:J:689:MET:HE1	1:J:719:ILE:N	2.01	0.74
1:J:236:ILE:HG13	1:J:712:HIS:CD2	2.22	0.74
1:J:360:SER:O	1:J:373:LYS:HE2	1.87	0.74
1:J:70:TYR:O	1:J:77:LEU:HD23	1.87	0.74
1:I:392:LYS:HE3	1:I:392:LYS:CA	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:289:ALA:CB	1:J:290:PRO:CA	2.66	0.74
1:J:431:LEU:HD23	1:J:470:LEU:HD21	1.69	0.74
1:I:438:ASP:OD2	1:I:441:LYS:HD3	1.88	0.73
1:J:286:GLN:NE2	1:J:288:THR:HG22	2.03	0.73
1:J:389:ILE:CG1	1:J:390:ASP:H	1.98	0.73
1:J:596:ARG:O	1:J:597:ARG:HD2	1.89	0.73
1:I:127:SER:HB3	1:I:211:TYR:CD1	2.23	0.73
1:J:221:THR:HB	1:J:274:ASP:OD2	1.87	0.73
1:J:289:ALA:HB1	1:J:290:PRO:C	2.12	0.73
1:J:674:PRO:O	1:J:680:LEU:HD13	1.88	0.73
1:J:385:CYS:HB3	1:J:387:PHE:HE2	1.51	0.73
1:I:107:ILE:CG1	1:I:114:ILE:HG12	2.11	0.73
1:J:383:HIS:ND1	1:J:398:THR:CG2	2.51	0.73
1:I:571:GLU:OE2	1:I:760:LYS:HD3	1.89	0.73
1:J:159:PRO:HG3	1:J:217:SER:O	1.87	0.73
1:I:674:PRO:C	1:I:680:LEU:HB2	2.14	0.73
1:I:484:SER:O	1:I:488:ASP:N	2.21	0.72
1:J:154:TRP:NE1	1:J:156:THR:HG23	2.04	0.72
1:I:542:LEU:C	1:I:542:LEU:HD23	2.15	0.72
1:I:139:LYS:HD3	1:I:141:GLN:HB2	1.70	0.72
1:I:150:ASN:O	1:I:151:ASN:HB2	1.89	0.72
1:I:103:ASN:HD21	1:I:120:TYR:HB2	1.54	0.72
1:I:153:GLN:HE22	1:I:170:ASN:ND2	1.88	0.72
1:I:155:VAL:HG22	1:I:156:THR:N	2.03	0.72
1:I:184:ARG:HH11	1:I:187:TRP:HA	1.55	0.72
1:J:314:GLN:HG3	1:J:325:MET:HG2	1.71	0.72
1:J:542:LEU:C	1:J:542:LEU:HD23	2.15	0.72
1:I:144:THR:O	1:I:147:ARG:HD2	1.89	0.71
1:I:515:ASP:CG	1:I:516:PHE:H	1.97	0.71
1:I:581:ARG:HG3	1:I:593:ALA:CB	2.20	0.71
1:J:109:PRO:HG2	1:J:158:SER:O	1.91	0.71
1:J:391:LYS:HD2	1:J:392:LYS:N	2.05	0.71
1:J:242:SER:HB3	1:J:246:LEU:HD12	1.72	0.71
1:J:611:ARG:HG3	1:J:611:ARG:NH1	2.04	0.71
1:I:289:ALA:CB	1:I:290:PRO:CA	2.67	0.71
1:I:118:TYR:HD2	1:I:119:ASN:OD1	1.72	0.71
1:J:160:VAL:HG12	1:J:161:GLY:N	2.04	0.71
1:J:487:ASN:HD21	1:J:489:LYS:HB3	1.54	0.70
1:I:276:LEU:CD2	1:I:276:LEU:H	2.03	0.70
1:I:370:SER:HB2	1:I:387:PHE:O	1.92	0.70
1:J:147:ARG:HG3	1:J:147:ARG:HH11	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:626:ILE:HD13	1:I:639:VAL:CG2	2.19	0.69
1:J:322:TYR:HD1	1:J:348:MET:HE3	1.57	0.69
1:J:214:LEU:HD12	1:J:214:LEU:O	1.92	0.69
1:J:516:PHE:CD2	1:J:523:LYS:HB2	2.27	0.69
1:I:96:ASP:CG	1:I:97:GLU:N	2.50	0.69
1:J:383:HIS:CE1	1:J:398:THR:HG22	2.26	0.69
1:J:755:MET:O	1:J:759:ILE:HG12	1.93	0.69
1:I:111:GLY:O	1:I:137:LEU:HD12	1.92	0.69
1:I:613:PHE:O	1:I:616:MET:HB2	1.93	0.69
1:J:159:PRO:HD3	1:J:216:TRP:CB	2.23	0.69
1:I:708:ASP:OD2	1:I:740:HIS:HA	1.93	0.69
1:I:158:SER:HB3	1:I:163:LYS:HB2	1.74	0.68
1:I:320:GLN:OE1	1:I:669:ARG:HD3	1.92	0.68
1:J:85:ASN:HD21	2:J:767:NAG:C2	2.05	0.68
1:I:267:LYS:HD3	4:I:784:HOH:O	1.93	0.68
1:I:93:SER:O	1:I:94:THR:C	2.36	0.68
1:I:415:LEU:HD13	1:I:415:LEU:C	2.19	0.68
1:J:156:THR:HG21	4:J:942:HOH:O	1.94	0.68
1:J:346:ILE:HD12	1:J:346:ILE:N	2.08	0.68
1:I:119:ASN:O	1:I:121:VAL:HG23	1.93	0.68
1:I:729:ASP:OD1	1:J:754:HIS:ND1	2.24	0.68
1:I:281:ASN:O	1:I:282:ALA:C	2.37	0.67
1:I:293:MET:CE	1:I:317:ARG:HG3	2.25	0.67
1:J:62:TRP:CE3	1:J:462:SER:HB3	2.28	0.67
1:J:518:ILE:HD13	1:J:523:LYS:HB3	1.75	0.67
1:I:333:SER:O	1:I:334:SER:HB2	1.94	0.67
1:I:313:LEU:HD12	1:I:313:LEU:N	2.10	0.67
1:J:229:ASN:HD21	2:J:771:NAG:H2	1.59	0.67
1:J:110:ASP:OD2	1:J:162:HIS:HB3	1.93	0.67
1:I:571:GLU:O	1:I:573:ILE:HG13	1.95	0.67
1:J:433:LYS:HG2	1:J:443:THR:CG2	2.26	0.66
1:J:657:SER:N	1:J:715:GLN:OE1	2.26	0.66
1:I:350:THR:O	1:I:350:THR:HG22	1.95	0.66
1:J:326:ASP:OD1	1:J:344:GLN:HG2	1.96	0.66
1:J:516:PHE:HD2	1:J:523:LYS:HB2	1.59	0.66
1:J:77:LEU:HA	1:J:89:PHE:H	1.60	0.65
1:J:598:LEU:HD23	1:J:659:TRP:CZ2	2.29	0.65
1:I:145:GLU:OE1	1:I:145:GLU:N	2.25	0.65
1:I:748:HIS:CE1	1:I:752:TYR:CE2	2.85	0.65
1:I:332:GLU:OE2	1:I:332:GLU:HA	1.96	0.65
1:J:72:GLN:HB3	1:J:75:ASN:OD1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:453:ARG:HA	4:J:925:HOH:O	1.96	0.65
1:I:276:LEU:H	1:I:276:LEU:HD23	1.60	0.65
1:I:410:LEU:HD13	1:I:415:LEU:CD2	2.23	0.65
1:J:55:LEU:CD2	1:J:500:LEU:HD23	2.27	0.65
1:I:293:MET:CE	1:I:293:MET:HA	2.27	0.65
1:I:232:GLU:HB3	1:I:262:VAL:HG11	1.79	0.65
1:I:352:GLY:HA2	1:I:595:ASN:ND2	2.11	0.65
1:J:65:ASP:HB2	1:J:463:LYS:HB2	1.77	0.65
1:J:120:TYR:HA	1:J:130:ALA:HB2	1.78	0.65
1:J:160:VAL:CG1	1:J:161:GLY:N	2.60	0.65
1:J:320:GLN:OE1	1:J:669:ARG:HD3	1.96	0.65
1:I:65:ASP:OD1	1:I:464:GLU:N	2.30	0.64
1:J:154:TRP:CE2	1:J:212:SER:HB2	2.32	0.64
1:J:268:PHE:CD2	1:J:313:LEU:HD21	2.32	0.64
1:J:114:ILE:HG22	1:J:137:LEU:CD2	2.26	0.64
1:I:293:MET:HE2	1:I:317:ARG:HG3	1.80	0.64
1:I:508:GLN:O	1:I:532:PRO:HG2	1.98	0.64
1:J:236:ILE:HG13	1:J:712:HIS:CE1	2.32	0.64
1:J:484:SER:O	1:J:488:ASP:HA	1.98	0.64
1:I:218:PRO:HB2	1:I:308:GLN:HG3	1.79	0.64
1:J:80:ASN:OD1	1:J:82:GLU:HB3	1.97	0.64
1:J:385:CYS:HB3	1:J:387:PHE:CE2	2.32	0.64
1:J:765:LEU:HD12	1:J:765:LEU:O	1.98	0.64
1:I:422:TYR:CD2	1:I:423:LYS:HD3	2.33	0.64
1:J:454:CYS:HA	1:J:474:GLY:O	1.98	0.64
1:J:318:ARG:NH1	1:J:668:GLU:OE2	2.30	0.64
1:J:321:ASN:ND2	2:J:774:NAG:N2	2.44	0.64
1:I:76:ILE:O	1:I:89:PHE:HB3	1.98	0.63
1:I:148:ILE:HG23	1:I:149:PRO:HD2	1.80	0.63
1:J:318:ARG:NH1	1:J:664:SER:HB2	2.10	0.63
1:J:318:ARG:NH1	1:J:668:GLU:CD	2.56	0.63
1:J:712:HIS:HB3	4:J:799:HOH:O	1.97	0.63
1:J:526:TYR:HE2	1:J:528:MET:CE	2.10	0.63
1:I:293:MET:HA	1:I:293:MET:HE2	1.80	0.63
1:I:516:PHE:CD2	1:I:523:LYS:HE3	2.34	0.63
1:I:614:SER:C	1:I:616:MET:H	2.06	0.63
1:J:229:ASN:ND2	2:J:771:NAG:C1	2.57	0.63
1:I:237:GLU:OE2	1:I:253:ARG:CD	2.45	0.63
1:I:635:VAL:O	1:I:639:VAL:HG22	1.98	0.63
1:J:154:TRP:HE1	1:J:156:THR:CG2	2.11	0.63
1:J:143:ILE:CD1	1:J:178:PRO:HB2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:272:ASN:HD22	1:I:273:THR:N	1.96	0.63
1:I:408:GLU:HG3	1:I:459:VAL:HG12	1.81	0.63
1:I:614:SER:HA	1:I:619:VAL:HB	1.81	0.63
1:J:741:GLY:O	1:J:742:ILE:C	2.39	0.63
1:J:658:ARG:CB	1:J:687:THR:HG22	2.29	0.62
1:I:203:TYR:CZ	1:I:228:PHE:HE1	2.17	0.62
1:J:136:ASP:HB3	1:J:139:LYS:CG	2.25	0.62
1:J:571:GLU:OE1	1:J:571:GLU:HA	1.99	0.62
1:I:97:GLU:O	1:I:98:PHE:HB2	1.98	0.62
1:I:734:TRP:CD1	1:I:734:TRP:C	2.77	0.62
1:I:741:GLY:O	1:I:742:ILE:C	2.41	0.62
1:J:154:TRP:HE1	1:J:156:THR:HG23	1.64	0.62
1:I:191:GLU:O	1:I:192:ASP:OD2	2.16	0.62
1:I:353:TRP:CZ2	1:I:591:MET:HE3	2.34	0.62
1:J:526:TYR:HB3	1:J:578:PHE:HD1	1.63	0.62
1:I:159:PRO:HD3	1:I:216:TRP:CB	2.29	0.62
1:I:190:LYS:O	1:I:193:ILE:HB	2.00	0.62
1:J:85:ASN:ND2	2:J:767:NAG:C1	2.63	0.61
1:J:98:PHE:HE1	1:J:102:ILE:HD11	1.65	0.61
1:I:134:ILE:O	1:I:142:LEU:HD12	2.00	0.61
1:J:77:LEU:N	1:J:77:LEU:CD2	2.63	0.61
1:J:318:ARG:NH1	1:J:668:GLU:OE1	2.34	0.61
1:I:139:LYS:O	1:I:141:GLN:N	2.33	0.61
1:I:289:ALA:HB1	1:I:290:PRO:C	2.26	0.61
1:I:429:ARG:HB2	1:I:456:TYR:HA	1.81	0.61
1:J:153:GLN:HE22	1:J:170:ASN:HD22	1.48	0.61
1:J:71:LYS:HA	1:J:76:ILE:HA	1.82	0.61
1:I:751:ILE:CG1	1:I:755:MET:HE2	2.26	0.61
1:J:471:ARG:HD3	1:J:480:TYR:HE2	1.64	0.61
1:J:671:MET:HE1	1:J:682:HIS:CD2	2.36	0.61
1:J:154:TRP:NE1	1:J:156:THR:CG2	2.63	0.61
1:J:614:SER:HB2	1:J:621:ASN:OD1	2.01	0.61
1:I:177:GLU:HB2	1:I:180:LEU:HG	1.83	0.61
1:I:331:ASP:O	1:I:332:GLU:C	2.43	0.61
1:J:401:THR:HG22	1:J:401:THR:O	2.00	0.61
1:I:74:ASN:O	1:I:92:ASN:CB	2.48	0.61
1:I:89:PHE:CE1	1:I:114:ILE:HD11	2.34	0.61
1:I:314:GLN:NE2	1:I:373:LYS:NZ	2.45	0.61
1:I:660:GLU:HG3	4:I:945:HOH:O	2.00	0.61
1:J:82:GLU:CG	1:J:83:TYR:CE1	2.83	0.61
1:J:331:ASP:CG	1:J:333:SER:HG	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:PHE:CE1	1:I:116:LEU:HD11	2.36	0.61
1:I:500:LEU:HG	1:I:504:LEU:CD1	2.30	0.61
1:J:127:SER:HB3	1:J:211:TYR:CD1	2.36	0.60
1:J:159:PRO:HD3	1:J:216:TRP:HB3	1.82	0.60
1:I:312:SER:C	1:I:313:LEU:HD12	2.27	0.60
1:I:118:TYR:CD2	1:I:119:ASN:OD1	2.54	0.60
1:J:640:LEU:HD11	1:J:650:GLY:HA3	1.83	0.60
1:J:153:GLN:HE22	1:J:170:ASN:ND2	2.00	0.60
1:J:500:LEU:HD12	1:J:503:MET:HE3	1.81	0.60
1:I:139:LYS:HD3	1:I:141:GLN:CB	2.31	0.60
1:J:438:ASP:OD2	1:J:441:LYS:HG3	2.00	0.60
1:I:155:VAL:CG2	1:I:156:THR:N	2.64	0.60
1:J:55:LEU:HD23	1:J:500:LEU:HD23	1.84	0.60
1:J:598:LEU:HG	1:J:631:TYR:OH	2.01	0.60
1:I:123:GLN:HG2	1:I:124:TRP:H	1.67	0.60
1:J:62:TRP:CZ3	1:J:462:SER:HB3	2.37	0.60
1:J:78:VAL:HG13	1:J:89:PHE:CB	2.25	0.60
1:J:596:ARG:O	1:J:597:ARG:CD	2.49	0.60
1:J:217:SER:CB	1:J:222:PHE:HB2	2.32	0.59
1:J:616:MET:HE2	1:J:618:PHE:CZ	2.37	0.59
1:I:291:ALA:O	1:I:295:ILE:HG23	2.03	0.59
1:I:664:SER:HB2	1:I:668:GLU:OE2	2.03	0.59
1:J:159:PRO:CD	1:J:216:TRP:HB3	2.33	0.59
1:J:376:SER:HA	1:J:382:ARG:HA	1.85	0.59
1:I:310:ARG:CD	1:I:329:ASP:OD1	2.41	0.59
1:J:500:LEU:HA	1:J:503:MET:HE2	1.84	0.59
1:I:528:MET:HE3	1:I:574:ILE:CG2	2.30	0.59
1:I:95:PHE:CZ	1:I:116:LEU:HD11	2.38	0.59
1:J:87:SER:HB2	2:J:767:NAG:H81	1.84	0.59
1:I:113:PHE:CZ	1:I:178:PRO:HG2	2.38	0.59
1:J:236:ILE:HD13	1:J:237:GLU:N	2.18	0.59
1:J:139:LYS:HG3	1:J:141:GLN:HB2	1.83	0.59
1:J:418:ILE:HG21	1:J:429:ARG:HG2	1.84	0.59
1:I:596:ARG:N	1:I:670:TYR:O	2.36	0.59
1:I:113:PHE:CE1	1:I:178:PRO:HG2	2.38	0.58
1:I:459:VAL:CG2	1:I:461:PHE:CE1	2.86	0.58
1:I:581:ARG:CG	1:I:593:ALA:CB	2.81	0.58
1:I:321:ASN:C	1:I:321:ASN:HD22	2.10	0.58
1:I:107:ILE:HD11	1:I:114:ILE:HD13	1.86	0.58
1:I:219:ASN:CG	1:I:308:GLN:HG2	2.27	0.58
1:I:135:TYR:OH	1:I:140:ARG:HD2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:600:THR:O	1:I:604:GLU:HG3	2.04	0.58
1:I:658:ARG:HG2	4:I:945:HOH:O	2.03	0.58
1:J:183:TYR:OH	1:J:277:SER:HA	2.03	0.58
1:J:598:LEU:HD23	1:J:659:TRP:CE2	2.38	0.58
1:I:81:ALA:O	1:I:491:LEU:HD13	2.03	0.58
1:J:88:VAL:CG1	1:J:91:GLU:HG2	2.34	0.58
1:J:110:ASP:OD2	1:J:162:HIS:ND1	2.36	0.58
1:I:133:ASP:HB3	1:I:142:LEU:HD11	1.85	0.58
1:I:703:ILE:HG12	1:I:733:MET:HB3	1.84	0.58
1:I:459:VAL:HG22	1:I:460:SER:N	2.18	0.58
1:J:147:ARG:HG3	1:J:147:ARG:NH1	2.17	0.58
1:J:345:HIS:HE1	1:J:389:ILE:HA	1.68	0.58
1:I:508:GLN:O	1:I:532:PRO:CG	2.52	0.58
1:J:461:PHE:CD2	1:J:468:TYR:HB3	2.39	0.58
1:I:88:VAL:HG11	1:I:91:GLU:HG2	1.84	0.58
1:I:242:SER:CB	1:I:246:LEU:HD12	2.33	0.58
1:I:573:ILE:HD11	1:I:765:LEU:HD11	1.86	0.58
1:J:276:LEU:O	1:J:277:SER:C	2.47	0.58
1:J:297:ASP:CB	1:J:318:ARG:HG3	2.34	0.58
1:J:461:PHE:CD2	1:J:465:ALA:HB1	2.39	0.58
1:J:526:TYR:CE2	1:J:528:MET:CE	2.86	0.58
1:I:148:ILE:HD11	1:I:164:LEU:CD2	2.34	0.57
1:I:661:TYR:OH	1:I:718:GLN:HG2	2.03	0.57
1:J:489:LYS:CE	1:J:491:LEU:HD21	2.19	0.57
1:I:134:ILE:C	1:I:143:ILE:HD13	2.29	0.57
1:J:516:PHE:CD2	1:J:523:LYS:HE3	2.38	0.57
1:I:517:ILE:HG23	1:I:526:TYR:CE2	2.39	0.57
1:I:616:MET:HE2	1:I:618:PHE:CZ	2.39	0.57
1:I:85:ASN:HD21	2:I:767:NAG:C2	2.17	0.57
1:I:696:LYS:HG2	1:I:728:VAL:HG22	1.85	0.57
1:J:345:HIS:CE1	1:J:389:ILE:HA	2.39	0.57
1:J:689:MET:HE1	1:J:719:ILE:HA	1.86	0.57
1:I:384:ILE:HG13	1:I:404:VAL:HG21	1.86	0.57
1:I:510:PRO:HD3	1:I:569:SER:HB2	1.85	0.57
1:J:229:ASN:ND2	2:J:771:NAG:H2	2.19	0.57
1:J:528:MET:HG2	1:J:576:ALA:HB2	1.85	0.57
1:J:95:PHE:CZ	1:J:116:LEU:HD11	2.39	0.57
1:J:664:SER:O	1:J:668:GLU:HB2	2.03	0.57
1:I:374:ILE:HD11	1:I:406:GLY:HA2	1.87	0.57
1:I:429:ARG:HG2	1:I:429:ARG:HH11	1.70	0.57
1:I:563:TRP:CE2	1:I:567:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:LEU:HD23	1:J:137:LEU:N	2.19	0.57
1:J:118:TYR:CD2	1:J:119:ASN:ND2	2.72	0.57
1:J:314:GLN:HG2	1:J:325:MET:HG2	1.84	0.57
1:J:334:SER:O	1:J:336:ARG:HG2	2.04	0.57
1:I:246:LEU:HD22	1:I:248:TYR:O	2.04	0.56
1:J:76:ILE:HD12	1:J:105:TYR:CE2	2.40	0.56
1:I:76:ILE:HD11	1:I:105:TYR:CD2	2.41	0.56
1:I:363:HIS:HE1	1:I:407:ILE:O	1.88	0.56
1:J:125:ARG:HG2	1:J:126:HIS:CE1	2.39	0.56
1:I:195:TYR:CE2	1:I:200:ASP:HA	2.39	0.56
1:I:204:GLU:O	1:I:209:SER:HA	2.04	0.56
1:I:214:LEU:O	1:I:214:LEU:HD12	2.06	0.56
1:I:272:ASN:C	1:I:272:ASN:ND2	2.56	0.56
1:I:644:SER:C	1:I:646:VAL:H	2.14	0.56
1:J:58:TYR:CE2	1:J:494:LEU:HB3	2.39	0.56
1:J:207:VAL:HG22	1:J:208:PHE:N	2.20	0.56
1:J:375:ILE:CD1	1:J:376:SER:O	2.52	0.56
1:J:689:MET:HE1	1:J:719:ILE:CA	2.36	0.56
1:J:377:ASN:C	1:J:377:ASN:ND2	2.58	0.56
1:J:553:GLN:HA	1:J:579:ASP:OD1	2.05	0.56
1:J:562:ASN:HD22	1:J:562:ASN:C	2.12	0.56
1:I:110:ASP:OD2	1:I:162:HIS:ND1	2.24	0.56
1:I:594:ILE:HD12	1:I:594:ILE:O	2.05	0.56
1:J:321:ASN:ND2	2:J:774:NAG:C2	2.69	0.56
1:I:65:ASP:OD2	1:I:466:LYS:HB2	2.06	0.56
2:J:769:NAG:O4	2:J:770:NAG:H2	2.05	0.56
1:I:139:LYS:O	1:I:139:LYS:HE2	2.06	0.56
1:J:45:LEU:HD22	1:J:49:LEU:CG	2.36	0.56
1:J:526:TYR:CE2	1:J:528:MET:HE3	2.31	0.56
1:I:573:ILE:HD11	1:I:765:LEU:CD1	2.36	0.56
1:I:676:PRO:HG2	1:I:677:GLU:OE2	2.06	0.56
1:J:415:LEU:C	1:J:415:LEU:HD23	2.31	0.56
1:J:459:VAL:HG22	1:J:460:SER:N	2.20	0.56
1:I:438:ASP:CG	1:I:441:LYS:HD3	2.31	0.56
1:J:272:ASN:C	1:J:272:ASN:HD22	2.12	0.56
1:I:594:ILE:HD12	1:I:594:ILE:C	2.32	0.55
1:J:99:GLY:C	1:J:100:HIS:ND1	2.64	0.55
1:J:415:LEU:HB2	1:J:436:LEU:HD11	1.88	0.55
1:I:159:PRO:CD	1:I:216:TRP:HB3	2.36	0.55
1:I:229:ASN:ND2	2:I:768:NAG:O5	2.39	0.55
1:J:581:ARG:NH2	1:J:605:ASP:OD1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:GLN:HE22	1:I:170:ASN:HD21	1.51	0.55
1:I:454:CYS:HB3	1:I:457:TYR:CZ	2.41	0.55
1:I:695:PHE:HB3	1:I:728:VAL:HG11	1.89	0.55
1:J:475:PRO:HA	1:J:557:THR:O	2.07	0.55
1:I:382:ARG:NH2	4:I:824:HOH:O	2.36	0.55
1:I:527:GLN:OE1	1:I:555:ALA:HA	2.06	0.55
1:I:581:ARG:HB2	1:I:605:ASP:OD2	2.06	0.55
1:I:651:ILE:HD11	1:I:758:PHE:HD2	1.70	0.55
1:J:258:LYS:NZ	1:J:712:HIS:CD2	2.68	0.55
1:I:546:VAL:CG2	1:I:547:TYR:N	2.69	0.55
1:J:197:GLY:C	1:J:213:ALA:HB3	2.32	0.55
1:J:272:ASN:HD22	1:J:274:ASP:H	1.54	0.55
1:J:302:ASP:OD1	1:J:304:THR:HG23	2.06	0.55
1:J:680:LEU:O	1:J:683:TYR:HB2	2.06	0.55
1:I:114:ILE:O	1:I:115:LEU:C	2.49	0.55
1:I:481:THR:OG1	1:I:483:HIS:HE1	1.89	0.55
1:J:358:ARG:HD3	3:J:1:JNH:H14	1.87	0.55
1:I:84:GLY:CA	1:I:492:ARG:NH2	2.69	0.55
1:I:691:ARG:HD2	4:I:820:HOH:O	2.05	0.55
1:J:173:TYR:HA	1:J:183:TYR:O	2.07	0.55
1:J:302:ASP:HB3	1:J:314:GLN:HB2	1.89	0.55
1:J:603:VAL:HG13	1:J:639:VAL:HG23	1.88	0.55
1:J:657:SER:HB2	1:J:689:MET:SD	2.47	0.55
1:I:107:ILE:HG22	1:I:108:SER:O	2.06	0.55
1:I:653:VAL:C	1:I:655:PRO:HD3	2.31	0.55
1:J:180:LEU:HB3	1:J:181:PRO:HD2	1.88	0.55
1:I:147:ARG:HG3	1:I:147:ARG:HH11	1.72	0.55
1:I:204:GLU:HB2	1:I:210:ALA:O	2.06	0.55
1:J:433:LYS:HG2	1:J:443:THR:HG23	1.88	0.55
1:J:453:ARG:NH2	1:J:477:LEU:O	2.34	0.54
1:I:105:TYR:CD1	1:I:106:SER:N	2.75	0.54
1:I:113:PHE:HB2	1:I:157:TRP:CH2	2.42	0.54
1:I:139:LYS:C	1:I:141:GLN:N	2.65	0.54
1:I:518:ILE:O	1:I:519:LEU:HD23	2.08	0.54
1:I:704:HIS:CD2	1:I:716:SER:OG	2.60	0.54
1:J:55:LEU:HD13	1:J:478:PRO:HG2	1.88	0.54
1:J:633:GLY:CA	1:J:655:PRO:HB3	2.36	0.54
1:I:281:ASN:O	1:I:282:ALA:O	2.24	0.54
1:I:146:GLU:O	1:I:147:ARG:C	2.48	0.54
1:J:55:LEU:HD23	1:J:500:LEU:CD2	2.38	0.54
1:I:124:TRP:HA	1:I:124:TRP:CE3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:45:LEU:CD2	1:J:49:LEU:HG	2.36	0.54
1:J:158:SER:HB3	1:J:163:LYS:HB2	1.89	0.54
1:J:658:ARG:HB3	1:J:687:THR:HG22	1.90	0.54
1:I:472:CYS:O	1:I:478:PRO:HA	2.08	0.54
1:J:146:GLU:HB3	1:J:175:LYS:NZ	2.23	0.54
1:I:79:PHE:CD1	1:I:86:SER:HB3	2.43	0.54
1:I:398:THR:HA	4:I:836:HOH:O	2.07	0.54
1:I:456:TYR:HB2	1:I:557:THR:OG1	2.08	0.54
1:I:674:PRO:O	1:I:680:LEU:HD13	2.06	0.54
1:J:518:ILE:HA	1:J:522:THR:O	2.08	0.54
1:I:155:VAL:CG2	1:I:156:THR:H	2.21	0.54
1:J:388:GLN:O	1:J:390:ASP:N	2.41	0.54
1:I:377:ASN:HB3	1:I:379:GLU:H	1.72	0.54
1:I:528:MET:HE1	1:I:618:PHE:CE1	2.43	0.54
1:J:87:SER:HB2	2:J:767:NAG:O7	2.08	0.54
1:J:477:LEU:HD23	1:J:501:ASP:HB2	1.89	0.54
1:I:614:SER:HB2	1:I:621:ASN:ND2	2.23	0.54
1:I:671:MET:CE	1:I:682:HIS:HD2	2.12	0.54
1:J:45:LEU:HD22	1:J:49:LEU:CD1	2.38	0.54
1:J:58:TYR:CD2	1:J:494:LEU:HB3	2.43	0.54
1:J:65:ASP:CG	1:J:464:GLU:H	2.15	0.54
1:J:659:TRP:HB3	1:J:667:THR:CG2	2.38	0.54
1:I:208:PHE:O	1:I:209:SER:C	2.52	0.53
1:I:314:GLN:HE22	1:I:373:LYS:HZ2	1.50	0.53
1:J:60:LEU:N	1:J:60:LEU:HD12	2.21	0.53
1:J:310:ARG:NH1	1:J:329:ASP:OD2	2.40	0.53
1:J:391:LYS:HD2	1:J:392:LYS:O	2.07	0.53
1:I:54:ARG:HG2	1:I:54:ARG:HH11	1.72	0.53
1:I:704:HIS:HD2	1:I:716:SER:OG	1.90	0.53
1:J:388:GLN:HG2	4:J:930:HOH:O	2.08	0.53
1:I:76:ILE:HD11	1:I:105:TYR:CE2	2.43	0.53
1:J:51:ASN:OD1	1:J:54:ARG:HG3	2.08	0.53
1:I:248:TYR:CZ	1:J:234:PRO:HB2	2.44	0.53
1:I:581:ARG:HG2	1:I:593:ALA:HB1	1.91	0.53
1:J:62:TRP:CH2	1:J:467:TYR:HB2	2.44	0.53
1:J:293:MET:HG2	1:J:315:TRP:HB3	1.89	0.53
1:J:546:VAL:CG2	1:J:547:TYR:N	2.70	0.53
1:I:438:ASP:OD2	1:I:441:LYS:CD	2.56	0.53
1:I:693:GLU:OE1	1:I:726:VAL:HG13	2.08	0.53
1:J:272:ASN:ND2	1:J:274:ASP:H	2.07	0.53
1:I:45:LEU:N	1:I:566:TYR:CD1	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:310:ARG:HH22	1:I:369:ASN:ND2	2.06	0.53
1:J:616:MET:HE2	1:J:618:PHE:HZ	1.73	0.53
1:I:72:GLN:O	1:I:73:GLU:HB2	2.08	0.53
1:I:47:ASP:HA	1:I:52:THR:OG1	2.08	0.53
1:I:495:GLU:OE2	1:I:497:ASN:N	2.37	0.53
1:J:76:ILE:HG12	1:J:90:LEU:HB3	1.91	0.53
1:I:155:VAL:HG22	1:I:156:THR:H	1.74	0.52
1:I:504:LEU:HD22	1:I:509:MET:SD	2.49	0.52
1:I:520:ASN:O	1:I:521:GLU:HB2	2.08	0.52
1:I:66:HIS:CE1	1:I:466:LYS:HZ2	2.27	0.52
1:I:229:ASN:HD21	2:I:768:NAG:C1	2.22	0.52
1:I:742:ILE:O	1:I:742:ILE:HG22	2.08	0.52
1:I:293:MET:HG3	1:I:298:HIS:CB	2.39	0.52
1:I:640:LEU:HD11	1:I:650:GLY:CA	2.30	0.52
1:J:95:PHE:CE1	1:J:116:LEU:HD11	2.44	0.52
1:I:107:ILE:CD1	1:I:114:ILE:HG23	2.31	0.52
1:I:128:TYR:CD1	1:I:128:TYR:C	2.88	0.52
1:I:203:TYR:CE2	1:I:228:PHE:HE1	2.28	0.52
1:J:118:TYR:O	1:J:119:ASN:HB2	2.08	0.52
1:I:123:GLN:HG2	1:I:124:TRP:N	2.25	0.52
1:I:204:GLU:CG	1:I:205:GLU:N	2.73	0.52
1:I:276:LEU:HD23	1:I:276:LEU:N	2.24	0.52
1:I:333:SER:O	1:I:334:SER:CB	2.57	0.52
1:J:131:SER:C	1:J:132:TYR:CD1	2.88	0.52
1:I:234:PRO:HB2	1:J:248:TYR:CZ	2.45	0.52
1:I:358:ARG:HD3	3:I:1:JNH:H14	1.91	0.52
1:I:750:HIS:CD2	1:J:724:VAL:HG22	2.45	0.52
1:I:190:LYS:O	1:I:191:GLU:C	2.53	0.52
1:I:454:CYS:HA	1:I:474:GLY:O	2.10	0.52
1:J:136:ASP:CG	1:J:139:LYS:HG2	2.34	0.52
1:I:219:ASN:ND2	1:I:308:GLN:HG2	2.25	0.52
1:I:408:GLU:HG3	1:I:459:VAL:HG11	1.88	0.52
1:J:114:ILE:HG22	1:J:135:TYR:O	2.10	0.52
1:J:146:GLU:OE2	1:J:146:GLU:HA	2.10	0.52
1:I:61:ARG:HH21	1:I:71:LYS:NZ	2.07	0.51
1:J:217:SER:O	1:J:218:PRO:C	2.53	0.51
1:I:134:ILE:HD11	1:I:164:LEU:HD22	1.93	0.51
1:I:345:HIS:HB3	4:I:795:HOH:O	2.09	0.51
1:I:654:ALA:HA	1:I:704:HIS:CD2	2.45	0.51
1:I:654:ALA:N	1:I:655:PRO:CD	2.73	0.51
1:J:106:SER:C	1:J:114:ILE:HD12	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:204:GLU:O	1:J:209:SER:HA	2.10	0.51
1:J:346:ILE:N	1:J:346:ILE:CD1	2.74	0.51
1:J:614:SER:HA	1:J:619:VAL:CB	2.37	0.51
1:J:179:ASN:OD1	1:J:180:LEU:N	2.43	0.51
1:I:66:HIS:CE1	1:I:466:LYS:NZ	2.78	0.51
1:I:526:TYR:CD1	1:I:526:TYR:C	2.87	0.51
1:J:676:PRO:HD3	1:J:680:LEU:HD22	1.91	0.51
1:I:105:TYR:HD1	1:I:106:SER:N	2.09	0.51
1:I:123:GLN:CG	1:I:124:TRP:N	2.73	0.51
1:I:146:GLU:OE2	1:I:146:GLU:HA	2.11	0.51
1:I:293:MET:CE	1:I:293:MET:CA	2.89	0.51
1:I:596:ARG:HA	1:I:670:TYR:O	2.11	0.51
1:J:273:THR:HA	1:J:276:LEU:HG	1.91	0.51
1:J:70:TYR:O	1:J:77:LEU:CD2	2.56	0.51
1:J:321:ASN:CG	2:J:774:NAG:C1	2.84	0.51
1:J:735:TYR:OH	1:J:751:ILE:HA	2.11	0.51
1:J:297:ASP:HB2	1:J:318:ARG:HG3	1.92	0.51
1:I:127:SER:O	1:I:128:TYR:HB3	2.11	0.51
1:I:58:TYR:CD2	1:I:494:LEU:HB3	2.46	0.51
1:I:63:ILE:HG21	1:I:69:LEU:HG	1.93	0.51
1:I:72:GLN:HB3	1:I:77:LEU:CD1	2.40	0.51
1:I:377:ASN:ND2	1:I:383:HIS:HD2	2.08	0.51
1:J:56:LYS:N	1:J:497:ASN:OD1	2.39	0.50
1:J:658:ARG:HG3	1:J:661:TYR:CD2	2.47	0.50
1:J:701:LEU:HD22	1:J:703:ILE:HG13	1.93	0.50
1:I:664:SER:O	1:I:665:VAL:C	2.55	0.50
1:I:693:GLU:HA	1:I:726:VAL:HG11	1.93	0.50
1:J:229:ASN:ND2	2:J:771:NAG:O5	2.45	0.50
1:J:484:SER:OG	1:J:489:LYS:HE2	2.12	0.50
1:I:113:PHE:CD1	1:I:134:ILE:CG2	2.94	0.50
1:I:305:TRP:CE2	1:I:311:ILE:HD12	2.47	0.50
1:J:410:LEU:HD12	1:J:411:THR:N	2.27	0.50
1:I:105:TYR:CE1	1:I:107:ILE:HD13	2.46	0.50
1:I:136:ASP:OD1	1:I:139:LYS:N	2.45	0.50
1:I:147:ARG:HD3	1:I:147:ARG:N	2.27	0.50
1:I:215:TRP:CZ2	1:I:303:VAL:HG21	2.46	0.50
1:I:528:MET:HG2	1:I:576:ALA:HB2	1.94	0.50
1:I:113:PHE:HD1	1:I:134:ILE:CG2	2.25	0.50
1:I:382:ARG:HH21	1:I:591:MET:HE1	1.77	0.50
1:J:382:ARG:NH2	4:J:782:HOH:O	2.45	0.50
1:J:471:ARG:HD3	1:J:480:TYR:CE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:509:MET:HE1	1:I:561:LEU:HD11	1.94	0.50
1:J:361:GLU:OE1	1:J:361:GLU:N	2.34	0.50
1:I:64:SER:HA	1:I:463:LYS:HG3	1.94	0.49
1:I:124:TRP:HA	1:I:124:TRP:HE3	1.76	0.49
1:I:146:GLU:O	1:I:147:ARG:O	2.30	0.49
1:I:317:ARG:O	1:I:318:ARG:C	2.54	0.49
1:I:478:PRO:HB2	1:I:497:ASN:ND2	2.27	0.49
1:J:658:ARG:HB2	1:J:687:THR:HG22	1.94	0.49
1:I:76:ILE:O	1:I:76:ILE:HG22	2.12	0.49
1:I:316:LEU:HD21	1:I:320:GLN:HG2	1.93	0.49
1:I:677:GLU:CD	1:I:677:GLU:H	2.21	0.49
1:J:55:LEU:CD2	1:J:500:LEU:CD2	2.90	0.49
1:J:128:TYR:CD1	1:J:128:TYR:C	2.90	0.49
1:J:236:ILE:CG1	1:J:712:HIS:CD2	2.95	0.49
1:J:388:GLN:O	1:J:389:ILE:HG12	2.11	0.49
1:J:431:LEU:HD12	1:J:432:TYR:N	2.27	0.49
1:I:314:GLN:NE2	1:I:373:LYS:HZ2	2.07	0.49
1:I:328:CYS:HA	1:I:338:ASN:O	2.11	0.49
1:I:631:TYR:H	3:I:1:JNH:C20	2.19	0.49
1:I:694:ASN:O	1:I:697:GLN:HG2	2.12	0.49
1:J:760:LYS:HE3	4:J:866:HOH:O	2.12	0.49
1:I:114:ILE:HG13	1:I:137:LEU:HD21	1.93	0.49
1:I:193:ILE:HG22	1:I:194:ILE:N	2.27	0.49
1:I:429:ARG:HB2	1:I:457:TYR:H	1.77	0.49
1:I:484:SER:O	1:I:488:ASP:CA	2.60	0.49
1:J:272:ASN:HB3	4:J:874:HOH:O	2.11	0.49
1:J:516:PHE:HA	1:J:525:TRP:HA	1.95	0.49
1:J:546:VAL:HG22	1:J:547:TYR:N	2.26	0.49
1:J:656:VAL:HA	1:J:715:GLN:OE1	2.12	0.49
1:J:658:ARG:HD2	1:J:661:TYR:CE1	2.47	0.49
1:I:139:LYS:C	1:I:141:GLN:H	2.21	0.49
1:I:148:ILE:HD11	1:I:164:LEU:HD21	1.94	0.49
1:I:344:GLN:O	1:I:392:LYS:HE2	2.13	0.49
1:I:392:LYS:CA	1:I:392:LYS:CE	2.88	0.49
1:I:514:LEU:CD2	1:I:514:LEU:C	2.85	0.49
1:I:536:LYS:NZ	1:I:536:LYS:CB	2.76	0.49
1:J:114:ILE:CG2	1:J:137:LEU:CD2	2.88	0.49
1:J:123:GLN:HG2	1:J:124:TRP:CD2	2.47	0.49
1:J:157:TRP:O	1:J:216:TRP:NE1	2.45	0.49
1:I:95:PHE:CE2	1:I:116:LEU:HD21	2.47	0.49
1:I:676:PRO:CD	1:I:677:GLU:OE2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:ASP:HA	1:J:52:THR:OG1	2.13	0.49
1:J:278:SER:OG	1:J:279:VAL:N	2.43	0.49
1:I:415:LEU:C	1:I:415:LEU:CD1	2.84	0.49
1:I:608:GLU:O	1:I:612:GLN:HG3	2.13	0.49
1:J:206:GLU:HB3	1:J:665:VAL:CG1	2.43	0.49
1:J:608:GLU:O	1:J:611:ARG:HB2	2.12	0.49
1:I:520:ASN:N	1:I:520:ASN:HD22	2.09	0.49
1:I:551:CYS:HA	1:I:584:GLY:N	2.28	0.49
1:J:102:ILE:HG22	1:J:104:ASP:H	1.77	0.49
1:J:288:THR:O	1:J:289:ALA:O	2.30	0.49
1:I:134:ILE:HG21	1:I:178:PRO:HB3	1.95	0.49
1:I:139:LYS:O	1:I:139:LYS:CE	2.60	0.49
1:I:150:ASN:O	1:I:151:ASN:CB	2.57	0.49
1:I:200:ASP:OD1	1:I:203:TYR:HB2	2.13	0.49
1:I:638:MET:HE1	4:I:820:HOH:O	2.13	0.49
1:J:160:VAL:CG1	1:J:161:GLY:H	2.25	0.49
1:J:372:TYR:OH	1:J:436:LEU:HG	2.12	0.49
1:I:84:GLY:HA3	1:I:492:ARG:NH2	2.28	0.49
1:I:95:PHE:CZ	1:I:135:TYR:CD2	3.00	0.49
1:I:658:ARG:HG3	1:I:687:THR:HG22	1.95	0.49
1:J:377:ASN:ND2	1:J:379:GLU:H	2.11	0.49
1:I:139:LYS:HD3	1:I:139:LYS:O	2.13	0.48
1:I:682:HIS:HA	1:I:685:ASN:HB2	1.95	0.48
1:I:184:ARG:HD2	1:I:187:TRP:CD2	2.48	0.48
1:I:310:ARG:HD2	1:I:327:ILE:HG22	1.94	0.48
1:J:465:ALA:O	1:J:485:SER:OG	2.30	0.48
1:J:603:VAL:HG13	1:J:639:VAL:CG2	2.43	0.48
1:I:440:THR:OG1	1:I:441:LYS:HD2	2.13	0.48
1:I:739:ASP:HB2	4:I:829:HOH:O	2.13	0.48
1:I:68:TYR:CD1	1:I:68:TYR:C	2.92	0.48
1:I:92:ASN:OD1	1:I:93:SER:N	2.45	0.48
1:I:266:VAL:HG22	1:I:267:LYS:N	2.28	0.48
1:I:316:LEU:CD2	1:I:320:GLN:HG2	2.43	0.48
1:I:542:LEU:C	1:I:542:LEU:CD2	2.86	0.48
1:I:660:GLU:CG	4:I:945:HOH:O	2.59	0.48
1:J:711:VAL:CG2	1:J:740:HIS:CE1	2.96	0.48
1:I:114:ILE:HG13	1:I:137:LEU:HD11	1.95	0.48
1:I:581:ARG:HG3	1:I:593:ALA:HB3	1.96	0.48
1:I:666:TYR:CZ	3:I:1:JNH:H41	2.48	0.48
1:J:232:GLU:HB2	1:J:262:VAL:HG11	1.96	0.48
1:J:450:ASN:OD1	1:J:453:ARG:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:TRP:CE2	1:I:169:ASN:OD1	2.66	0.48
1:I:480:TYR:CD1	1:I:480:TYR:N	2.82	0.48
1:I:658:ARG:HB3	1:I:661:TYR:CD2	2.48	0.48
1:J:375:ILE:HD12	1:J:376:SER:O	2.13	0.48
1:J:562:ASN:ND2	1:J:565:THR:H	2.12	0.48
1:I:614:SER:C	1:I:616:MET:N	2.69	0.48
1:J:103:ASN:O	1:J:104:ASP:HB2	2.13	0.48
1:J:171:ASP:HB3	1:J:173:TYR:CE1	2.49	0.48
1:J:229:ASN:HB3	1:J:265:THR:OG1	2.14	0.48
1:J:407:ILE:HG23	1:J:415:LEU:HD21	1.96	0.48
1:I:112:GLN:C	1:I:113:PHE:CD2	2.92	0.48
1:I:229:ASN:CG	2:I:768:NAG:O5	2.56	0.48
1:J:659:TRP:HB3	1:J:667:THR:HG21	1.95	0.48
1:I:148:ILE:HD11	1:I:164:LEU:HD23	1.96	0.48
1:I:436:LEU:CD1	1:I:436:LEU:N	2.76	0.48
1:I:581:ARG:CG	1:I:593:ALA:HB1	2.42	0.48
1:I:743:ALA:O	1:I:744:SER:C	2.54	0.48
1:J:53:TYR:HB3	1:J:500:LEU:HD11	1.94	0.48
1:J:418:ILE:CG2	1:J:429:ARG:HG2	2.43	0.48
1:I:49:LEU:HD13	1:I:749:GLN:HG2	1.96	0.48
1:I:327:ILE:HD13	1:I:389:ILE:HG22	1.95	0.48
1:I:689:MET:HE3	1:J:244:GLU:HG3	1.95	0.48
1:J:533:HIS:O	1:J:535:ASP:N	2.47	0.48
1:J:592:HIS:HE1	4:J:805:HOH:O	1.97	0.48
1:J:687:THR:HB	1:J:689:MET:HG2	1.95	0.48
1:I:216:TRP:CZ3	1:I:220:GLY:O	2.67	0.47
1:I:242:SER:O	1:J:721:LYS:NZ	2.46	0.47
1:J:600:THR:OG1	1:J:601:PHE:N	2.40	0.47
1:I:229:ASN:HD21	2:I:768:NAG:H2	1.76	0.47
1:I:738:GLU:OE2	1:I:747:ALA:HB2	2.14	0.47
1:I:63:ILE:CG2	1:I:69:LEU:HG	2.45	0.47
1:I:184:ARG:HD2	1:I:187:TRP:CE2	2.49	0.47
1:J:459:VAL:CG2	1:J:460:SER:N	2.77	0.47
1:J:513:LYS:O	1:J:527:GLN:HA	2.14	0.47
1:J:544:LEU:HD21	1:J:606:GLN:HE21	1.79	0.47
1:I:80:ASN:O	1:I:84:GLY:HA2	2.15	0.47
1:I:703:ILE:HA	1:I:733:MET:O	2.14	0.47
1:J:43:TYR:O	1:J:566:TYR:HA	2.15	0.47
1:J:376:SER:HA	1:J:381:TYR:O	2.13	0.47
1:J:662:TYR:HB3	1:J:667:THR:OG1	2.14	0.47
1:I:177:GLU:HB2	1:I:180:LEU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:ALA:HA	1:I:294:LEU:HD11	1.96	0.47
1:I:701:LEU:HD22	1:I:703:ILE:HG13	1.96	0.47
1:J:171:ASP:OD1	1:J:184:ARG:NH1	2.48	0.47
1:J:177:GLU:HB2	1:J:180:LEU:HG	1.95	0.47
1:J:431:LEU:CD2	1:J:470:LEU:HD21	2.39	0.47
1:I:60:LEU:C	1:I:60:LEU:HD12	2.39	0.47
1:I:80:ASN:O	1:I:84:GLY:N	2.47	0.47
1:I:129:THR:HG22	1:I:153:GLN:HA	1.96	0.47
1:I:153:GLN:O	1:I:154:TRP:HB2	2.15	0.47
1:I:268:PHE:C	1:I:269:PHE:CD1	2.93	0.47
1:I:293:MET:HE2	1:I:317:ARG:CG	2.43	0.47
1:J:114:ILE:HG23	1:J:114:ILE:O	2.14	0.47
1:J:314:GLN:HE22	1:J:373:LYS:CE	2.27	0.47
1:I:76:ILE:CD1	1:I:105:TYR:CE2	2.98	0.47
1:I:274:ASP:N	1:I:276:LEU:HD22	2.30	0.47
1:J:50:LYS:O	1:J:51:ASN:C	2.58	0.47
1:J:388:GLN:O	1:J:389:ILE:CG1	2.63	0.47
1:J:434:ILE:HG23	1:J:434:ILE:O	2.14	0.47
1:J:484:SER:HB2	1:J:489:LYS:HG2	1.97	0.47
1:I:308:GLN:HE21	1:I:308:GLN:HB2	1.55	0.47
1:I:383:HIS:HB3	1:I:398:THR:OG1	2.15	0.47
1:I:674:PRO:HA	1:I:683:TYR:CD2	2.49	0.47
1:J:71:LYS:C	1:J:73:GLU:H	2.22	0.47
1:J:297:ASP:HB3	1:J:318:ARG:CG	2.45	0.47
1:J:448:GLU:O	1:J:449:LEU:C	2.57	0.47
1:J:107:ILE:HG12	1:J:108:SER:N	2.30	0.47
1:J:114:ILE:HG21	1:J:135:TYR:HD2	1.80	0.47
1:J:408:GLU:HG3	1:J:459:VAL:CG1	2.45	0.47
1:I:74:ASN:O	1:I:92:ASN:CA	2.64	0.46
1:I:316:LEU:HG	1:I:320:GLN:HG2	1.96	0.46
1:I:470:LEU:HA	1:I:470:LEU:HD23	1.63	0.46
1:J:386:TYR:CE2	1:J:388:GLN:NE2	2.83	0.46
1:J:578:PHE:CD2	1:J:609:ALA:HB2	2.50	0.46
1:J:689:MET:HE1	1:J:718:GLN:O	2.14	0.46
1:I:216:TRP:HZ3	1:I:220:GLY:O	1.98	0.46
1:I:304:THR:HB	1:I:312:SER:OG	2.14	0.46
1:I:704:HIS:CE1	1:I:713:PHE:HA	2.50	0.46
1:J:223:LEU:HD13	1:J:223:LEU:C	2.40	0.46
1:J:726:VAL:HG23	1:J:728:VAL:HG23	1.97	0.46
1:I:418:ILE:HA	1:I:430:ASN:O	2.15	0.46
1:J:77:LEU:HB2	1:J:87:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:95:PHE:O	1:J:98:PHE:HB2	2.16	0.46
1:J:256:TYR:CD1	1:J:256:TYR:C	2.94	0.46
1:J:429:ARG:O	1:J:457:TYR:N	2.48	0.46
1:J:516:PHE:HE2	1:J:518:ILE:HD11	1.78	0.46
1:I:365:THR:HG22	1:I:366:LEU:N	2.31	0.46
1:J:127:SER:HA	1:J:211:TYR:HB2	1.96	0.46
1:J:559:PHE:C	1:J:559:PHE:CD2	2.93	0.46
1:I:146:GLU:HG3	1:I:181:PRO:N	2.30	0.46
1:I:158:SER:CB	1:I:163:LYS:HB2	2.44	0.46
1:I:301:CYS:SG	1:I:359:PRO:CG	3.03	0.46
1:I:429:ARG:HG2	1:I:429:ARG:NH1	2.29	0.46
1:J:571:GLU:CD	1:J:760:LYS:HD3	2.41	0.46
1:I:422:TYR:CZ	1:I:423:LYS:HD3	2.50	0.46
1:J:46:THR:O	1:J:50:LYS:HB2	2.16	0.46
1:J:65:ASP:OD2	1:J:466:LYS:HG3	2.15	0.46
1:J:125:ARG:HB3	4:J:780:HOH:O	2.14	0.46
1:I:738:GLU:OE2	1:I:744:SER:HB3	2.15	0.46
1:J:105:TYR:HB2	1:J:114:ILE:HD11	1.98	0.46
1:J:250:LYS:NZ	1:J:250:LYS:HB3	2.31	0.46
1:J:413:ASP:HB3	1:J:414:TYR:HD1	1.80	0.46
1:J:110:ASP:OD2	1:J:162:HIS:CG	2.69	0.46
1:J:321:ASN:ND2	2:J:774:NAG:C1	2.78	0.46
1:I:105:TYR:CD1	1:I:105:TYR:C	2.93	0.46
1:I:197:GLY:C	1:I:213:ALA:HB3	2.41	0.46
1:I:500:LEU:O	1:I:501:ASP:C	2.59	0.46
1:J:113:PHE:CZ	1:J:178:PRO:HG2	2.51	0.46
1:J:314:GLN:NE2	1:J:373:LYS:HE3	2.30	0.46
1:I:203:TYR:CE2	1:I:228:PHE:CE1	3.04	0.46
1:I:204:GLU:O	1:I:209:SER:CA	2.63	0.46
1:I:281:ASN:HD21	2:I:770:NAG:H62	1.80	0.46
1:I:314:GLN:HE22	1:I:373:LYS:HZ1	1.58	0.46
1:I:675:THR:HG21	4:I:900:HOH:O	2.15	0.46
1:J:518:ILE:HD13	1:J:523:LYS:CB	2.44	0.46
1:J:689:MET:CE	1:J:719:ILE:HA	2.46	0.46
1:I:84:GLY:HA3	1:I:492:ARG:CZ	2.46	0.45
1:I:107:ILE:HG13	1:I:114:ILE:CD1	2.46	0.45
1:I:294:LEU:C	1:I:296:GLY:N	2.74	0.45
1:I:321:ASN:C	1:I:321:ASN:ND2	2.74	0.45
1:I:436:LEU:N	1:I:436:LEU:HD12	2.30	0.45
1:J:293:MET:HG3	1:J:298:HIS:CB	2.47	0.45
1:J:622:LYS:C	1:J:623:ARG:HG3	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:659:TRP:CE3	1:J:667:THR:HG23	2.50	0.45
1:J:689:MET:CE	1:J:718:GLN:C	2.78	0.45
1:I:127:SER:CB	1:I:211:TYR:CD1	2.95	0.45
1:I:143:ILE:HD12	1:I:143:ILE:N	2.32	0.45
1:I:403:GLU:OE1	1:I:585:TYR:HA	2.16	0.45
1:I:536:LYS:HZ3	1:I:536:LYS:HB3	1.81	0.45
1:J:397:ILE:HG22	1:J:439:TYR:CZ	2.51	0.45
1:J:562:ASN:HD22	1:J:565:THR:H	1.64	0.45
1:J:48:TYR:CD1	1:J:562:ASN:HA	2.51	0.45
1:I:115:LEU:HD21	1:I:155:VAL:HG11	1.98	0.45
1:I:229:ASN:HD21	2:I:768:NAG:C2	2.30	0.45
1:I:269:PHE:CE2	1:I:286:GLN:HB2	2.52	0.45
1:J:83:TYR:CD1	1:J:83:TYR:N	2.84	0.45
1:J:257:PRO:O	1:J:663:ASP:HA	2.16	0.45
1:I:215:TRP:CH2	1:I:303:VAL:HG21	2.51	0.45
1:I:290:PRO:HG2	1:I:324:VAL:HG11	1.98	0.45
1:I:626:ILE:HB	1:I:647:PHE:CE2	2.51	0.45
1:J:219:ASN:ND2	2:J:769:NAG:O5	2.49	0.45
1:J:358:ARG:HD3	3:J:1:JNH:C14	2.46	0.45
1:J:477:LEU:CD2	1:J:501:ASP:HB2	2.47	0.45
1:J:487:ASN:CG	1:J:489:LYS:HB3	2.41	0.45
1:I:82:GLU:HG2	1:I:83:TYR:CE1	2.52	0.45
1:J:134:ILE:HG21	1:J:178:PRO:HB3	1.99	0.45
1:J:219:ASN:ND2	1:J:221:THR:CG2	2.64	0.45
1:J:375:ILE:HD11	1:J:376:SER:O	2.17	0.45
1:J:623:ARG:HB3	1:J:763:PHE:CD1	2.51	0.45
1:I:441:LYS:HD2	1:I:441:LYS:N	2.31	0.45
1:J:377:ASN:N	1:J:381:TYR:O	2.42	0.45
1:I:267:LYS:CB	1:I:269:PHE:HE1	2.24	0.45
1:J:616:MET:HB3	1:J:618:PHE:CE2	2.52	0.45
1:J:662:TYR:OH	3:J:1:JNH:H42	2.16	0.45
1:J:739:ASP:O	1:J:741:GLY:N	2.49	0.45
1:I:115:LEU:HG	1:I:132:TYR:HD2	1.82	0.45
1:I:170:ASN:ND2	1:I:198:ILE:HD11	2.31	0.45
1:I:301:CYS:SG	1:I:359:PRO:HG2	2.57	0.45
1:I:484:SER:O	1:I:488:ASP:HA	2.17	0.45
1:I:496:ASP:CG	1:I:498:SER:HG	2.23	0.45
1:I:614:SER:O	1:I:616:MET:N	2.48	0.45
1:I:748:HIS:CE1	1:I:752:TYR:HE2	2.32	0.45
1:J:173:TYR:CE2	1:J:184:ARG:HG2	2.51	0.45
1:J:293:MET:HE3	1:J:315:TRP:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:675:THR:OG1	1:J:677:GLU:HG2	2.17	0.45
1:J:690:SER:HB3	4:J:816:HOH:O	2.17	0.45
1:I:93:SER:O	1:I:95:PHE:N	2.50	0.45
1:I:515:ASP:CG	1:I:516:PHE:N	2.65	0.45
1:J:174:VAL:O	1:J:182:SER:HA	2.17	0.45
1:I:55:LEU:N	1:I:55:LEU:CD1	2.80	0.44
1:I:204:GLU:HG3	1:I:205:GLU:N	2.28	0.44
1:I:422:TYR:C	1:I:424:GLY:H	2.25	0.44
1:J:78:VAL:CG1	1:J:89:PHE:CD2	3.00	0.44
1:I:361:GLU:OE1	1:I:361:GLU:N	2.40	0.44
1:I:387:PHE:CD2	1:I:394:CYS:HB3	2.51	0.44
1:J:114:ILE:CB	1:J:137:LEU:HD21	2.47	0.44
1:J:205:GLU:OE2	3:J:1:JNH:H6	2.17	0.44
1:J:675:THR:C	1:J:680:LEU:HB2	2.42	0.44
1:J:711:VAL:HG21	1:J:740:HIS:CE1	2.52	0.44
1:I:345:HIS:CE1	1:I:389:ILE:O	2.70	0.44
1:I:720:SER:O	1:I:724:VAL:HG23	2.18	0.44
1:J:69:LEU:HD21	1:J:78:VAL:HG12	2.00	0.44
1:J:310:ARG:HD3	1:J:327:ILE:HG23	1.98	0.44
1:J:422:TYR:CE1	1:J:447:CYS:HB3	2.52	0.44
1:J:535:ASP:OD2	1:J:535:ASP:C	2.60	0.44
1:I:147:ARG:HG3	1:I:147:ARG:NH1	2.32	0.44
1:I:293:MET:CA	1:I:293:MET:HE3	2.46	0.44
1:I:661:TYR:CZ	1:I:718:GLN:HG2	2.53	0.44
2:J:767:NAG:H61	2:J:768:NAG:O7	2.16	0.44
1:I:369:ASN:HA	1:I:389:ILE:HD13	1.99	0.44
1:I:597:ARG:HA	1:I:682:HIS:NE2	2.32	0.44
1:I:626:ILE:O	1:I:650:GLY:HA2	2.18	0.44
1:I:658:ARG:CG	4:I:945:HOH:O	2.62	0.44
1:I:708:ASP:OD1	1:I:711:VAL:N	2.51	0.44
1:I:507:VAL:O	1:I:509:MET:N	2.42	0.44
1:J:146:GLU:HB3	1:J:175:LYS:HZ1	1.82	0.44
1:J:309:GLU:OE1	2:J:769:NAG:H61	2.17	0.44
1:J:495:GLU:OE2	1:J:497:ASN:N	2.50	0.44
1:J:512:LYS:HE2	1:J:556:ASP:O	2.18	0.44
1:J:530:LEU:HA	1:J:531:PRO:HD3	1.89	0.44
1:I:194:ILE:CD1	1:I:229:ASN:OD1	2.66	0.44
1:J:100:HIS:CD2	1:J:118:TYR:CE2	3.06	0.44
1:J:280:THR:HG22	1:J:281:ASN:N	2.33	0.44
1:J:736:THR:O	1:J:737:ASP:HB2	2.17	0.44
1:I:258:LYS:HD2	1:J:247:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:273:THR:O	1:I:274:ASP:OD1	2.35	0.44
1:I:679:ASN:O	1:I:680:LEU:C	2.60	0.44
1:J:96:ASP:C	1:J:98:PHE:N	2.76	0.44
1:J:120:TYR:HE1	1:J:128:TYR:CD2	2.36	0.44
1:J:271:VAL:HG22	1:J:272:ASN:N	2.33	0.44
1:J:330:TYR:HB2	1:J:337:TRP:CH2	2.52	0.44
1:J:472:CYS:O	1:J:478:PRO:HA	2.17	0.44
1:J:568:ALA:HA	1:J:573:ILE:O	2.18	0.44
1:J:750:HIS:HA	4:J:971:HOH:O	2.17	0.44
1:I:199:THR:HB	1:I:203:TYR:HB3	2.00	0.44
1:I:207:VAL:HG12	1:I:208:PHE:N	2.33	0.44
1:J:61:ARG:HB3	1:J:69:LEU:HB2	2.00	0.44
1:J:235:LEU:HA	1:J:254:VAL:O	2.18	0.44
1:J:236:ILE:O	1:J:236:ILE:CG2	2.64	0.44
1:J:290:PRO:HD3	1:J:315:TRP:CD1	2.53	0.44
1:J:626:ILE:O	1:J:650:GLY:HA2	2.18	0.44
1:I:55:LEU:N	1:I:55:LEU:HD12	2.33	0.43
1:I:571:GLU:O	1:I:572:ASN:C	2.58	0.43
1:I:596:ARG:O	1:I:597:ARG:NH1	2.38	0.43
1:J:71:LYS:HG2	1:J:73:GLU:H	1.82	0.43
1:J:171:ASP:CB	1:J:173:TYR:HE1	2.31	0.43
1:J:703:ILE:HG12	1:J:733:MET:HB3	1.98	0.43
1:I:373:LYS:HE3	1:I:373:LYS:HB2	1.84	0.43
1:I:459:VAL:CG2	1:I:460:SER:N	2.81	0.43
1:I:644:SER:OG	1:I:646:VAL:HG23	2.17	0.43
1:J:134:ILE:N	1:J:134:ILE:HD13	2.32	0.43
1:J:288:THR:O	1:J:289:ALA:C	2.61	0.43
1:I:204:GLU:HA	1:I:210:ALA:O	2.18	0.43
1:I:326:ASP:CB	4:I:881:HOH:O	2.66	0.43
1:J:217:SER:O	1:J:219:ASN:N	2.51	0.43
1:J:697:GLN:C	1:J:698:VAL:CG1	2.91	0.43
1:I:562:ASN:O	1:I:565:THR:HB	2.18	0.43
1:I:143:ILE:CG2	1:I:144:THR:N	2.81	0.43
1:I:203:TYR:CD2	1:I:228:PHE:CE1	3.06	0.43
1:I:65:ASP:CG	1:I:464:GLU:HB2	2.44	0.43
1:I:214:LEU:HA	1:I:225:TYR:HA	2.01	0.43
1:I:345:HIS:CD2	4:I:795:HOH:O	2.71	0.43
1:I:377:ASN:ND2	1:I:383:HIS:CD2	2.85	0.43
1:I:397:ILE:HG13	1:I:398:THR:HG23	2.00	0.43
1:I:509:MET:O	1:I:532:PRO:HG3	2.18	0.43
1:I:516:PHE:CG	1:I:523:LYS:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:600:THR:N	1:I:602:GLU:OE2	2.51	0.43
1:I:741:GLY:C	1:I:743:ALA:N	2.74	0.43
1:J:48:TYR:CE1	1:J:562:ASN:HA	2.53	0.43
1:J:87:SER:HB2	2:J:767:NAG:C8	2.48	0.43
1:I:134:ILE:HG22	1:I:135:TYR:N	2.33	0.43
1:I:546:VAL:HG23	1:I:547:TYR:N	2.33	0.43
1:I:696:LYS:CG	1:I:728:VAL:HG22	2.48	0.43
1:I:701:LEU:C	1:I:701:LEU:CD2	2.92	0.43
1:J:207:VAL:HG22	1:J:208:PHE:CD2	2.53	0.43
1:J:397:ILE:HB	1:J:439:TYR:CD1	2.54	0.43
1:J:673:LEU:HB2	1:J:678:ASP:OD2	2.18	0.43
1:I:97:GLU:O	1:I:98:PHE:CB	2.65	0.43
1:I:139:LYS:O	1:I:139:LYS:CD	2.67	0.43
1:I:209:SER:HB2	3:I:1:JNH:C15	2.49	0.43
1:I:476:GLY:O	1:I:559:PHE:HB2	2.18	0.43
1:J:61:ARG:O	1:J:62:TRP:C	2.61	0.43
1:J:110:ASP:OD2	1:J:162:HIS:CB	2.63	0.43
1:J:167:VAL:HA	1:J:171:ASP:O	2.19	0.43
1:J:387:PHE:CD2	1:J:387:PHE:N	2.87	0.43
1:I:658:ARG:HB3	1:I:661:TYR:CE2	2.54	0.43
1:I:65:ASP:HB3	4:I:937:HOH:O	2.19	0.43
1:I:219:ASN:ND2	4:I:862:HOH:O	2.25	0.43
1:I:235:LEU:HD23	1:I:255:PRO:HA	2.00	0.43
1:I:247:GLN:NE2	4:I:833:HOH:O	2.45	0.43
1:I:256:TYR:CD1	1:I:256:TYR:C	2.97	0.43
1:I:535:ASP:CG	1:I:537:SER:HG	2.27	0.43
1:J:65:ASP:CA	1:J:462:SER:HB2	2.30	0.43
1:J:310:ARG:HD3	1:J:327:ILE:CG2	2.48	0.43
1:J:358:ARG:HD2	3:J:1:JNH:H15	2.01	0.43
1:I:608:GLU:OE1	1:I:608:GLU:HA	2.18	0.42
1:I:125:ARG:O	1:I:125:ARG:HG2	2.18	0.42
1:I:429:ARG:CB	1:I:457:TYR:H	2.32	0.42
1:I:481:THR:HB	1:I:483:HIS:CE1	2.54	0.42
1:J:43:TYR:CE2	1:J:565:THR:HB	2.54	0.42
1:J:223:LEU:HD13	1:J:223:LEU:O	2.19	0.42
1:J:242:SER:CB	1:J:246:LEU:HD12	2.44	0.42
1:J:358:ARG:CD	3:J:1:JNH:H15	2.48	0.42
1:J:504:LEU:HA	1:J:507:VAL:CG1	2.50	0.42
1:J:562:ASN:C	1:J:562:ASN:ND2	2.78	0.42
1:I:54:ARG:HG2	1:I:54:ARG:NH1	2.32	0.42
1:I:134:ILE:HG22	1:I:143:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:51:ASN:CG	1:J:54:ARG:HG3	2.43	0.42
1:J:90:LEU:HD21	1:J:95:PHE:HE2	1.84	0.42
1:J:254:VAL:HA	1:J:255:PRO:HD3	1.88	0.42
1:J:500:LEU:CD1	1:J:503:MET:HE3	2.46	0.42
1:I:58:TYR:CE2	1:I:494:LEU:HB3	2.55	0.42
1:I:64:SER:CA	1:I:463:LYS:HG3	2.49	0.42
1:I:267:LYS:HG3	1:I:286:GLN:HE22	1.84	0.42
1:I:329:ASP:OD2	1:I:343:ARG:NH1	2.53	0.42
1:I:535:ASP:OD2	1:I:535:ASP:C	2.63	0.42
1:I:701:LEU:HD23	1:I:702:LEU:N	2.34	0.42
1:J:55:LEU:HD21	1:J:500:LEU:HD23	1.97	0.42
1:J:60:LEU:HD13	1:J:469:GLN:CD	2.45	0.42
1:J:477:LEU:HA	1:J:477:LEU:HD12	1.80	0.42
1:J:608:GLU:O	1:J:609:ALA:C	2.62	0.42
1:I:72:GLN:OE1	1:I:72:GLN:HA	2.19	0.42
1:I:114:ILE:O	1:I:114:ILE:HG22	2.17	0.42
1:I:192:ASP:OD2	1:I:192:ASP:C	2.62	0.42
1:I:530:LEU:HA	1:I:531:PRO:HD3	1.85	0.42
1:J:206:GLU:CB	1:J:665:VAL:HG11	2.50	0.42
1:I:542:LEU:HD23	1:I:543:LEU:N	2.35	0.42
1:I:596:ARG:CA	1:I:670:TYR:O	2.67	0.42
1:I:716:SER:HA	1:I:719:ILE:HD12	2.02	0.42
1:J:256:TYR:CZ	1:J:663:ASP:HB3	2.55	0.42
1:J:340:LEU:C	1:J:342:ALA:N	2.76	0.42
1:J:510:PRO:HD3	1:J:569:SER:HB2	2.01	0.42
1:I:313:LEU:N	1:I:313:LEU:CD1	2.79	0.42
1:I:433:LYS:NZ	1:I:488:ASP:OD2	2.40	0.42
1:J:169:ASN:O	1:J:170:ASN:HB2	2.19	0.42
1:J:330:TYR:HB2	1:J:337:TRP:CZ3	2.55	0.42
1:J:456:TYR:HB2	1:J:557:THR:OG1	2.20	0.42
1:I:541:PRO:CG	1:I:573:ILE:HG12	2.49	0.42
1:I:601:PHE:O	1:I:602:GLU:C	2.63	0.42
1:I:620:ASP:O	1:I:621:ASN:C	2.62	0.42
1:J:250:LYS:NZ	1:J:250:LYS:CB	2.82	0.42
1:J:513:LYS:HD3	1:J:515:ASP:HB2	2.02	0.42
1:J:656:VAL:HA	1:J:715:GLN:CD	2.44	0.42
1:I:105:TYR:CD1	1:I:107:ILE:CD1	3.03	0.42
1:I:124:TRP:HB3	4:I:848:HOH:O	2.20	0.42
1:I:209:SER:HB2	3:I:1:JNH:C16	2.50	0.42
1:I:267:LYS:HG3	1:I:286:GLN:NE2	2.35	0.42
1:I:676:PRO:HD2	1:I:677:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:ASP:OD1	1:J:112:GLN:HB2	2.20	0.42
1:J:127:SER:CB	1:J:211:TYR:CD1	3.02	0.42
1:J:236:ILE:O	1:J:236:ILE:HG23	2.19	0.42
1:I:422:TYR:C	1:I:424:GLY:N	2.76	0.42
1:I:446:SER:O	1:I:447:CYS:C	2.62	0.42
1:I:600:THR:OG1	1:I:601:PHE:N	2.53	0.42
1:I:751:ILE:HG23	1:I:752:TYR:N	2.35	0.42
1:J:96:ASP:C	1:J:98:PHE:H	2.28	0.42
1:J:146:GLU:OE1	1:J:181:PRO:HB3	2.20	0.42
1:J:383:HIS:CD2	1:J:399:LYS:HA	2.55	0.42
1:J:469:GLN:CD	1:J:471:ARG:HE	2.26	0.42
1:J:554:LYS:HB3	1:J:577:SER:HB3	2.01	0.42
1:I:316:LEU:CG	1:I:320:GLN:HG2	2.50	0.41
1:I:341:VAL:O	1:I:344:GLN:HG2	2.19	0.41
1:I:429:ARG:HB2	1:I:457:TYR:N	2.35	0.41
1:I:612:GLN:O	1:I:613:PHE:C	2.62	0.41
1:J:159:PRO:HD3	1:J:216:TRP:HB2	2.00	0.41
1:J:318:ARG:HH12	1:J:664:SER:CB	2.20	0.41
1:J:627:TRP:HB2	1:J:651:ILE:HB	2.02	0.41
1:I:123:GLN:CG	1:I:124:TRP:H	2.27	0.41
1:I:625:ALA:HB2	1:I:649:CYS:SG	2.60	0.41
1:I:748:HIS:CE1	1:I:752:TYR:CD2	3.08	0.41
1:J:51:ASN:CG	1:J:51:ASN:O	2.63	0.41
1:J:69:LEU:HD23	1:J:69:LEU:HA	1.81	0.41
1:J:150:ASN:ND2	4:J:905:HOH:O	2.49	0.41
1:J:184:ARG:NH1	1:J:187:TRP:HA	2.35	0.41
1:J:272:ASN:HD21	1:J:274:ASP:HB2	1.85	0.41
1:J:743:ALA:C	1:J:744:SER:O	2.60	0.41
1:I:531:PRO:HA	1:I:532:PRO:HD3	1.93	0.41
2:I:767:NAG:H83	2:I:767:NAG:O3	2.20	0.41
1:J:113:PHE:CE2	1:J:178:PRO:HG2	2.56	0.41
1:J:297:ASP:HB3	1:J:318:ARG:HG3	2.03	0.41
1:J:331:ASP:OD2	1:J:333:SER:OG	2.34	0.41
1:J:496:ASP:O	1:J:497:ASN:C	2.63	0.41
1:I:421:GLU:O	1:I:422:TYR:C	2.63	0.41
1:J:281:ASN:ND2	2:J:773:NAG:C1	2.83	0.41
1:J:388:GLN:C	1:J:389:ILE:HG12	2.46	0.41
1:J:433:LYS:HE2	1:J:443:THR:HG21	2.02	0.41
1:I:612:GLN:O	1:I:615:LYS:N	2.54	0.41
1:J:227:GLN:O	1:J:266:VAL:HA	2.20	0.41
1:J:268:PHE:HD2	1:J:287:ILE:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:457:TYR:CE1	1:J:472:CYS:HB2	2.55	0.41
1:J:763:PHE:O	1:J:764:SER:C	2.64	0.41
1:I:145:GLU:C	1:I:147:ARG:H	2.29	0.41
1:I:551:CYS:HA	1:I:584:GLY:CA	2.51	0.41
1:J:174:VAL:O	1:J:183:TYR:N	2.54	0.41
1:I:425:MET:HA	1:I:426:PRO:HD2	1.96	0.41
1:I:657:SER:N	1:I:715:GLN:OE1	2.43	0.41
1:I:675:THR:HB	1:I:677:GLU:OE2	2.21	0.41
1:J:79:PHE:CE2	1:J:86:SER:HB2	2.55	0.41
1:J:246:LEU:HD23	1:J:246:LEU:HA	1.80	0.41
1:J:479:LEU:HD12	1:J:495:GLU:O	2.20	0.41
1:J:581:ARG:HB2	1:J:605:ASP:OD2	2.21	0.41
1:I:310:ARG:HD2	1:I:327:ILE:CG2	2.51	0.41
1:I:374:ILE:CG2	1:I:382:ARG:HB3	2.51	0.41
1:J:216:TRP:CZ3	1:J:220:GLY:O	2.73	0.41
1:J:535:ASP:N	1:J:540:TYR:OH	2.54	0.41
1:J:562:ASN:ND2	1:J:562:ASN:H	2.19	0.41
1:I:89:PHE:CD1	1:I:89:PHE:C	2.99	0.41
1:I:139:LYS:O	1:I:140:ARG:C	2.63	0.41
1:I:206:GLU:CD	3:I:1:JNH:HN22	2.29	0.41
1:I:269:PHE:CD1	1:I:269:PHE:N	2.89	0.41
1:I:523:LYS:HE3	1:I:523:LYS:HB2	1.82	0.41
1:I:566:TYR:CD2	1:I:567:LEU:N	2.89	0.41
1:I:666:TYR:O	1:I:670:TYR:CE2	2.74	0.41
1:I:673:LEU:C	1:I:675:THR:H	2.29	0.41
1:J:65:ASP:OD1	1:J:464:GLU:N	2.41	0.41
1:J:104:ASP:O	1:J:117:GLU:HB3	2.21	0.41
1:J:155:VAL:O	1:J:155:VAL:HG13	2.20	0.41
1:J:206:GLU:HG3	1:J:663:ASP:OD1	2.21	0.41
1:J:616:MET:CE	1:J:618:PHE:HZ	2.33	0.41
1:J:648:LYS:NZ	1:J:762:CYS:O	2.53	0.41
1:I:143:ILE:HG22	1:I:144:THR:N	2.35	0.41
1:I:482:LEU:O	1:I:491:LEU:N	2.50	0.41
1:J:58:TYR:HD1	1:J:60:LEU:CD1	2.34	0.41
1:J:170:ASN:HD22	1:J:170:ASN:N	2.19	0.41
1:J:314:GLN:CG	1:J:325:MET:CG	2.95	0.41
1:I:541:PRO:HG2	1:I:573:ILE:HG12	2.03	0.40
1:J:108:SER:HA	1:J:109:PRO:HD3	1.91	0.40
1:J:701:LEU:HA	1:J:731:GLN:O	2.21	0.40
1:I:183:TYR:HE1	1:I:277:SER:O	2.05	0.40
1:J:176:ILE:HD13	1:J:176:ILE:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:258:LYS:HZ1	1:J:712:HIS:CD2	2.17	0.40
1:J:360:SER:O	1:J:373:LYS:CE	2.65	0.40
1:J:207:VAL:CG2	1:J:208:PHE:N	2.80	0.40
1:J:386:TYR:CZ	1:J:388:GLN:NE2	2.89	0.40
1:J:542:LEU:C	1:J:542:LEU:CD2	2.87	0.40
1:J:668:GLU:HG2	1:J:672:GLY:O	2.22	0.40
1:J:711:VAL:HG23	1:J:740:HIS:CE1	2.55	0.40
1:I:44:THR:HA	1:I:566:TYR:HD1	1.86	0.40
1:I:107:ILE:HD12	1:I:114:ILE:CG2	2.38	0.40
1:I:621:ASN:HD22	1:I:621:ASN:HA	1.61	0.40
1:I:676:PRO:CG	1:I:677:GLU:OE2	2.68	0.40
1:J:118:TYR:CE1	1:J:131:SER:CB	3.05	0.40
1:J:203:TYR:CD2	1:J:207:VAL:HG11	2.55	0.40
1:J:206:GLU:CB	1:J:665:VAL:CG1	3.00	0.40
1:J:427:GLY:HA3	4:J:813:HOH:O	2.21	0.40
1:J:658:ARG:HB3	1:J:687:THR:CG2	2.51	0.40
1:I:679:ASN:O	1:I:681:ASP:N	2.54	0.40
1:J:206:GLU:OE2	3:J:1:JNH:N2	2.54	0.40
1:J:564:ALA:O	1:J:565:THR:C	2.65	0.40
1:J:649:CYS:HB3	1:J:699:GLU:HB2	2.03	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	I	724/728 (100%)	607 (84%)	86 (12%)	31 (4%)	2 2
1	J	726/728 (100%)	632 (87%)	82 (11%)	12 (2%)	7 13
All	All	1450/1456 (100%)	1239 (85%)	168 (12%)	43 (3%)	3 5

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	94	THR
1	I	98	PHE
1	I	99	GLY
1	I	140	ARG
1	I	147	ARG
1	I	282	ALA
1	I	289	ALA
1	I	332	GLU
1	J	74	ASN
1	J	289	ALA
1	J	534	PHE
1	I	104	ASP
1	I	334	SER
1	I	422	TYR
1	I	463	LYS
1	I	615	LYS
1	J	277	SER
1	J	320	GLN
1	J	389	ILE
1	J	740	HIS
1	I	191	GLU
1	I	274	ASP
1	I	423	LYS
1	I	447	CYS
1	I	464	GLU
1	J	423	LYS
1	J	506	ASN
1	I	73	GLU
1	I	360	SER
1	I	645	GLY
1	I	665	VAL
1	J	486	VAL
1	I	88	VAL
1	I	128	TYR
1	I	149	PRO
1	I	508	GLN
1	I	664	SER
1	I	680	LEU
1	J	497	ASN
1	I	357	PHE
1	J	451	PRO
1	I	193	ILE
1	I	114	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	651/653 (100%)	609 (94%)	42 (6%)	15	32
1	J	653/653 (100%)	604 (92%)	49 (8%)	12	26
All	All	1304/1306 (100%)	1213 (93%)	91 (7%)	14	29

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	54	ARG
1	I	74	ASN
1	I	139	LYS
1	I	144	THR
1	I	147	ARG
1	I	184	ARG
1	I	204	GLU
1	I	218	PRO
1	I	243	ASP
1	I	246	LEU
1	I	267	LYS
1	I	272	ASN
1	I	276	LEU
1	I	293	MET
1	I	308	GLN
1	I	313	LEU
1	I	321	ASN
1	I	341	VAL
1	I	385	CYS
1	I	388	GLN
1	I	392	LYS
1	I	415	LEU
1	I	442	VAL
1	I	486	VAL
1	I	487	ASN
1	I	502	LYS
1	I	506	ASN

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Mol	Chain	Res	Type
1	I	514	LEU
1	I	536	LYS
1	I	546	VAL
1	I	554	LYS
1	I	566	TYR
1	I	589	LYS
1	I	608	GLU
1	I	621	ASN
1	I	679	ASN
1	I	685	ASN
1	I	689	MET
1	I	697	GLN
1	I	701	LEU
1	I	702	LEU
1	I	718	GLN
1	J	45	LEU
1	J	77	LEU
1	J	100	HIS
1	J	107	ILE
1	J	137	LEU
1	J	184	ARG
1	J	207	VAL
1	J	221	THR
1	J	236	ILE
1	J	246	LEU
1	J	250	LYS
1	J	256	TYR
1	J	309	GLU
1	J	318	ARG
1	J	325	MET
1	J	326	ASP
1	J	327	ILE
1	J	346	ILE
1	J	375	ILE
1	J	377	ASN
1	J	378	GLU
1	J	385	CYS
1	J	387	PHE
1	J	429	ARG
1	J	436	LEU
1	J	443	THR
1	J	445	LEU

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Mol	Chain	Res	Type
1	J	463	LYS
1	J	477	LEU
1	J	486	VAL
1	J	505	GLN
1	J	507	VAL
1	J	508	GLN
1	J	513	LYS
1	J	543	LEU
1	J	554	LYS
1	J	562	ASN
1	J	598	LEU
1	J	611	ARG
1	J	612	GLN
1	J	627	TRP
1	J	658	ARG
1	J	673	LEU
1	J	689	MET
1	J	701	LEU
1	J	702	LEU
1	J	704	HIS
1	J	714	GLN
1	J	765	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	51	ASN
1	I	66	HIS
1	I	74	ASN
1	I	103	ASN
1	I	123	GLN
1	I	150	ASN
1	I	169	ASN
1	I	170	ASN
1	I	247	GLN
1	I	263	ASN
1	I	272	ASN
1	I	281	ASN
1	I	286	GLN
1	I	308	GLN
1	I	314	GLN
1	I	321	ASN

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Mol	Chain	Res	Type
1	I	338	ASN
1	I	345	HIS
1	I	369	ASN
1	I	377	ASN
1	I	455	GLN
1	I	483	HIS
1	I	487	ASN
1	I	505	GLN
1	I	506	ASN
1	I	508	GLN
1	I	520	ASN
1	I	595	ASN
1	I	612	GLN
1	I	621	ASN
1	I	679	ASN
1	I	694	ASN
1	I	697	GLN
1	I	704	HIS
1	I	748	HIS
1	J	85	ASN
1	J	112	GLN
1	J	119	ASN
1	J	123	GLN
1	J	126	HIS
1	J	150	ASN
1	J	169	ASN
1	J	170	ASN
1	J	219	ASN
1	J	229	ASN
1	J	272	ASN
1	J	281	ASN
1	J	286	GLN
1	J	314	GLN
1	J	321	ASN
1	J	338	ASN
1	J	344	GLN
1	J	345	HIS
1	J	369	ASN
1	J	377	ASN
1	J	435	GLN
1	J	508	GLN
1	J	562	ASN

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Mol	Chain	Res	Type
1	J	606	GLN
1	J	679	ASN
1	J	712	HIS
1	J	718	GLN
1	J	731	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](#)

16 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	NAG	I	770	-	14,14,15	2.72	2 (14%)	17,19,21	2.64	7 (41%)
2	NAG	J	769	-	14,14,15	2.76	2 (14%)	17,19,21	2.57	7 (41%)
2	NAG	I	768	-	14,14,15	2.72	3 (21%)	17,19,21	3.58	4 (23%)
2	NAG	J	768	-	14,14,15	2.79	3 (21%)	17,19,21	3.05	6 (35%)
2	NAG	J	774	-	14,14,15	2.79	3 (21%)	17,19,21	3.16	7 (41%)
2	NAG	J	773	-	14,14,15	2.98	3 (21%)	17,19,21	2.47	5 (29%)
2	NAG	J	772	-	14,14,15	2.75	2 (14%)	17,19,21	3.48	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	775	-	14,14,15	2.80	3 (21%)	17,19,21	2.82	8 (47%)
2	NAG	J	771	-	14,14,15	3.13	4 (28%)	17,19,21	5.89	7 (41%)
3	JNH	J	1	1	26,26,26	1.56	6 (23%)	34,35,35	2.06	8 (23%)
2	NAG	I	769	-	14,14,15	2.57	2 (14%)	17,19,21	2.08	5 (29%)
3	JNH	I	1	1	26,26,26	1.70	7 (26%)	34,35,35	1.56	7 (20%)
2	NAG	J	767	-	14,14,15	2.74	3 (21%)	17,19,21	3.06	10 (58%)
2	NAG	I	767	-	14,14,15	2.93	3 (21%)	17,19,21	2.33	5 (29%)
2	NAG	J	770	-	14,14,15	3.02	4 (28%)	17,19,21	2.50	7 (41%)
2	NAG	I	771	-	14,14,15	2.73	2 (14%)	17,19,21	1.78	5 (29%)

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	NAG	I	770	-	-	2/6/23/26	0/1/1/1
2	NAG	J	769	-	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	I	768	-	2/2/5/7	1/6/23/26	0/1/1/1
2	NAG	J	768	-	-	2/6/23/26	0/1/1/1
2	NAG	J	774	-	-	2/6/23/26	0/1/1/1
2	NAG	J	773	-	-	3/6/23/26	0/1/1/1
2	NAG	J	772	-	-	3/6/23/26	0/1/1/1
2	NAG	J	775	-	-	3/6/23/26	0/1/1/1
2	NAG	J	771	-	1/1/5/7	1/6/23/26	0/1/1/1
3	JNH	J	1	1	1/1/4/4	6/18/28/28	0/3/3/3
2	NAG	I	769	-	-	3/6/23/26	0/1/1/1
3	JNH	I	1	1	-	4/18/28/28	0/3/3/3
2	NAG	J	767	-	-	4/6/23/26	0/1/1/1
2	NAG	I	767	-	-	2/6/23/26	0/1/1/1
2	NAG	J	770	-	-	2/6/23/26	0/1/1/1
2	NAG	I	771	-	1/1/5/7	4/6/23/26	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	771	NAG	O7-C7	9.33	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	773	NAG	O7-C7	9.32	1.44	1.23
2	J	770	NAG	O7-C7	9.27	1.44	1.23
2	I	767	NAG	O7-C7	9.02	1.43	1.23
2	J	768	NAG	O7-C7	9.00	1.43	1.23
2	J	769	NAG	O7-C7	8.93	1.43	1.23
2	J	772	NAG	O7-C7	8.91	1.43	1.23
2	I	770	NAG	O7-C7	8.77	1.42	1.23
2	I	771	NAG	O7-C7	8.66	1.42	1.23
2	J	774	NAG	O7-C7	8.63	1.42	1.23
2	J	775	NAG	O7-C7	8.47	1.42	1.23
2	J	767	NAG	O7-C7	8.39	1.42	1.23
2	I	768	NAG	O7-C7	8.36	1.41	1.23
2	I	769	NAG	O7-C7	8.34	1.41	1.23
2	J	770	NAG	C7-N2	4.79	1.49	1.34
2	I	767	NAG	C7-N2	4.74	1.49	1.34
2	J	773	NAG	C7-N2	4.52	1.48	1.34
2	J	775	NAG	C7-N2	4.51	1.48	1.34
2	J	771	NAG	C7-N2	4.49	1.48	1.34
2	I	771	NAG	C7-N2	4.48	1.48	1.34
2	J	767	NAG	C7-N2	4.47	1.48	1.34
2	J	774	NAG	C7-N2	4.33	1.48	1.34
2	J	769	NAG	C7-N2	4.26	1.48	1.34
2	J	768	NAG	C7-N2	4.16	1.47	1.34
2	I	768	NAG	C7-N2	4.10	1.47	1.34
2	I	770	NAG	C7-N2	4.08	1.47	1.34
2	I	769	NAG	C7-N2	4.06	1.47	1.34
2	J	772	NAG	C7-N2	3.93	1.47	1.34
3	I	1	JNH	C20-N3	-3.86	1.29	1.48
2	J	771	NAG	C1-C2	-3.57	1.47	1.52
3	J	1	JNH	C20-N3	-3.20	1.32	1.48
3	I	1	JNH	C20-C1	-2.83	1.50	1.53
2	I	767	NAG	C8-C7	2.82	1.56	1.50
3	J	1	JNH	C17-C8	-2.70	1.42	1.49
2	J	767	NAG	C4-C5	2.69	1.58	1.53
2	J	770	NAG	C2-N2	2.57	1.50	1.46
3	I	1	JNH	C18-C17	2.48	1.44	1.39
3	I	1	JNH	C15-C16	2.47	1.43	1.38
3	J	1	JNH	C5-N1	2.47	1.40	1.34
3	I	1	JNH	C17-C8	-2.46	1.43	1.49
3	I	1	JNH	C4-N1	-2.45	1.42	1.47
2	J	771	NAG	C8-C7	2.30	1.55	1.50
3	J	1	JNH	C19-C18	2.26	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	JNH	C16-C17	2.21	1.43	1.39
3	J	1	JNH	C18-C17	2.20	1.43	1.39
2	J	775	NAG	C8-C7	2.15	1.55	1.50
3	J	1	JNH	C16-C17	2.15	1.43	1.39
2	J	770	NAG	C8-C7	2.10	1.54	1.50
2	J	773	NAG	C3-C2	2.10	1.56	1.52
2	J	774	NAG	O5-C1	-2.06	1.40	1.43
2	J	768	NAG	C8-C7	2.04	1.54	1.50
2	I	768	NAG	C4-C5	2.02	1.57	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	771	NAG	C2-N2-C7	-19.45	96.83	122.90
2	I	768	NAG	C2-N2-C7	-12.74	105.83	122.90
2	J	771	NAG	C1-O5-C5	-9.80	99.06	112.19
2	J	768	NAG	C2-N2-C7	-9.62	110.00	122.90
2	J	772	NAG	C2-N2-C7	-9.47	110.20	122.90
2	J	774	NAG	C2-N2-C7	-9.16	110.62	122.90
2	J	771	NAG	O5-C1-C2	-8.73	97.78	111.29
2	I	767	NAG	C2-N2-C7	-6.77	113.83	122.90
2	I	770	NAG	C2-N2-C7	-6.64	114.01	122.90
2	J	773	NAG	C2-N2-C7	-6.42	114.29	122.90
2	J	767	NAG	O7-C7-C8	-6.28	110.88	122.05
3	J	1	JNH	C20-C1-N1	6.24	132.16	110.64
2	J	772	NAG	C8-C7-N2	-6.22	105.80	116.12
2	J	775	NAG	C2-N2-C7	-5.66	115.31	122.90
2	J	775	NAG	O7-C7-C8	-5.59	112.09	122.05
2	J	770	NAG	O7-C7-C8	-5.43	112.38	122.05
2	I	769	NAG	O7-C7-C8	-5.37	112.49	122.05
2	J	772	NAG	O7-C7-C8	-5.34	112.54	122.05
2	J	770	NAG	C8-C7-N2	-5.32	107.29	116.12
2	J	775	NAG	C1-O5-C5	-5.27	105.12	112.19
2	J	768	NAG	C1-O5-C5	-5.13	105.31	112.19
2	J	774	NAG	C1-O5-C5	-5.06	105.40	112.19
2	I	770	NAG	O7-C7-C8	-5.01	113.13	122.05
2	J	769	NAG	C2-N2-C7	-5.00	116.20	122.90
2	J	769	NAG	C8-C7-N2	-4.77	108.21	116.12
2	I	767	NAG	O7-C7-C8	-4.73	113.62	122.05
2	J	767	NAG	C3-C4-C5	4.60	118.58	110.23
2	I	768	NAG	C8-C7-N2	-4.59	108.51	116.12
2	J	767	NAG	C2-N2-C7	-4.49	116.89	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	767	NAG	O3-C3-C2	4.45	118.64	109.40
3	J	1	JNH	C11-C7-C6	4.43	123.20	114.13
2	I	768	NAG	O7-C7-C8	-4.25	114.49	122.05
2	J	773	NAG	O7-C7-C8	-4.23	114.52	122.05
2	J	774	NAG	O4-C4-C3	-4.17	100.54	110.38
2	I	770	NAG	C8-C7-N2	-4.15	109.24	116.12
2	J	769	NAG	O7-C7-C8	-4.12	114.71	122.05
2	J	767	NAG	O4-C4-C3	-4.11	100.68	110.38
2	J	767	NAG	C1-O5-C5	-4.02	106.79	112.19
3	J	1	JNH	C7-C11-C12	-3.97	113.51	120.90
2	J	769	NAG	O3-C3-C4	-3.86	101.29	110.38
2	J	772	NAG	O5-C1-C2	-3.80	105.42	111.29
2	J	774	NAG	O7-C7-C8	-3.72	115.42	122.05
2	J	768	NAG	C8-C7-N2	-3.67	110.03	116.12
3	I	1	JNH	C20-C1-N1	3.67	123.29	110.64
2	J	773	NAG	C8-C7-N2	-3.65	110.06	116.12
3	I	1	JNH	C6-C5-N1	-3.51	111.78	118.74
2	I	771	NAG	O7-C7-C8	-3.39	116.01	122.05
2	J	773	NAG	C4-C3-C2	-3.39	106.05	111.02
2	I	769	NAG	C2-N2-C7	-3.33	118.44	122.90
3	J	1	JNH	C2-C1-C20	-3.25	100.03	112.17
2	J	769	NAG	O4-C4-C3	-3.24	102.74	110.38
2	J	772	NAG	C1-C2-N2	-3.22	105.35	110.43
2	I	769	NAG	C8-C7-N2	-3.18	110.85	116.12
2	J	772	NAG	C1-O5-C5	-3.17	107.94	112.19
3	J	1	JNH	C1-C20-N3	3.12	134.24	111.50
2	I	771	NAG	O7-C7-N2	3.04	127.34	121.98
2	J	775	NAG	C6-C5-C4	-3.02	105.61	113.02
2	I	771	NAG	C1-O5-C5	2.99	116.19	112.19
2	J	770	NAG	C2-N2-C7	2.96	126.86	122.90
2	J	775	NAG	C3-C4-C5	2.95	115.58	110.23
2	I	770	NAG	O5-C5-C6	2.95	113.40	107.66
2	J	770	NAG	O7-C7-N2	2.93	127.17	121.98
2	J	769	NAG	O5-C5-C6	2.81	113.13	107.66
3	J	1	JNH	C2-C3-C4	-2.76	97.21	104.90
2	J	774	NAG	C3-C4-C5	2.76	115.23	110.23
2	J	771	NAG	O7-C7-N2	2.74	126.82	121.98
3	I	1	JNH	O1-C5-C6	2.74	124.64	119.61
3	I	1	JNH	C1-C20-N3	2.71	131.28	111.50
2	J	768	NAG	C1-C2-N2	-2.70	106.17	110.43
2	J	767	NAG	O5-C1-C2	-2.69	107.13	111.29
2	J	770	NAG	C1-O5-C5	-2.65	108.63	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	768	NAG	C1-O5-C5	2.65	115.73	112.19
2	J	768	NAG	O7-C7-C8	-2.62	117.38	122.05
2	J	770	NAG	O3-C3-C4	-2.61	104.22	110.38
2	J	774	NAG	O6-C6-C5	2.61	120.22	111.33
2	J	775	NAG	C1-C2-N2	-2.61	106.32	110.43
2	J	775	NAG	O5-C1-C2	-2.60	107.26	111.29
2	J	771	NAG	C8-C7-N2	-2.60	111.81	116.12
3	I	1	JNH	C13-C12-C11	-2.52	117.69	121.00
2	J	769	NAG	O6-C6-C5	2.52	119.90	111.33
2	J	774	NAG	C4-C3-C2	2.46	114.63	111.02
2	I	769	NAG	C1-C2-N2	-2.43	106.61	110.43
2	J	771	NAG	O5-C5-C6	2.42	112.38	107.66
3	J	1	JNH	C7-C11-C10	2.37	125.32	120.90
3	I	1	JNH	C7-C6-C5	-2.36	103.11	109.43
2	I	771	NAG	C8-C7-N2	-2.35	112.22	116.12
2	J	775	NAG	C8-C7-N2	-2.34	112.24	116.12
2	I	770	NAG	O5-C1-C2	2.30	114.86	111.29
2	J	768	NAG	O5-C5-C6	2.25	112.05	107.66
3	I	1	JNH	C12-C11-C10	2.22	121.53	118.23
2	I	767	NAG	C4-C3-C2	-2.19	107.80	111.02
2	J	767	NAG	O5-C5-C6	2.19	111.93	107.66
3	J	1	JNH	C4-N1-C1	-2.15	107.65	111.44
2	J	770	NAG	O4-C4-C3	-2.15	105.30	110.38
2	I	771	NAG	C2-N2-C7	-2.15	120.02	122.90
2	J	771	NAG	O7-C7-C8	-2.11	118.29	122.05
2	I	770	NAG	O4-C4-C3	-2.11	105.40	110.38
2	I	767	NAG	C3-C4-C5	2.11	114.06	110.23
2	I	770	NAG	C3-C4-C5	2.10	114.05	110.23
2	I	769	NAG	O7-C7-N2	-2.10	118.28	121.98
2	J	773	NAG	C1-O5-C5	-2.08	109.40	112.19
2	I	767	NAG	C8-C7-N2	-2.07	112.68	116.12
2	J	767	NAG	C1-C2-N2	-2.06	107.18	110.43
2	J	767	NAG	O6-C6-C5	2.06	118.35	111.33

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	768	NAG	C5
2	I	768	NAG	C3
2	I	771	NAG	C5
2	J	769	NAG	C4
2	J	771	NAG	C3

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Mol	Chain	Res	Type	Atom
3	J	1	JNH	C6

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	767	NAG	C8-C7-N2-C2
2	I	767	NAG	O7-C7-N2-C2
2	I	768	NAG	C8-C7-N2-C2
2	I	769	NAG	C8-C7-N2-C2
2	I	769	NAG	O7-C7-N2-C2
2	I	770	NAG	C8-C7-N2-C2
2	I	770	NAG	O7-C7-N2-C2
2	J	767	NAG	C8-C7-N2-C2
2	J	770	NAG	C1-C2-N2-C7
2	J	772	NAG	O7-C7-N2-C2
2	J	773	NAG	O7-C7-N2-C2
2	J	774	NAG	O7-C7-N2-C2
2	J	775	NAG	C1-C2-N2-C7
2	J	775	NAG	C8-C7-N2-C2
2	J	775	NAG	O7-C7-N2-C2
3	I	1	JNH	N1-C1-C20-N3
3	I	1	JNH	C2-C1-C20-N3
3	J	1	JNH	N1-C1-C20-N3
2	J	767	NAG	O7-C7-N2-C2
2	J	767	NAG	O5-C5-C6-O6
2	J	773	NAG	O5-C5-C6-O6
2	J	772	NAG	O5-C5-C6-O6
2	J	773	NAG	C4-C5-C6-O6
2	I	771	NAG	C8-C7-N2-C2
2	J	771	NAG	O5-C5-C6-O6
2	J	769	NAG	O7-C7-N2-C2
2	J	770	NAG	O7-C7-N2-C2
3	J	1	JNH	C10-C11-C7-C6
2	J	768	NAG	O5-C5-C6-O6
3	J	1	JNH	C12-C11-C7-C6
2	J	772	NAG	C4-C5-C6-O6
2	J	767	NAG	C4-C5-C6-O6
3	J	1	JNH	C2-C1-C20-N3
2	I	769	NAG	O5-C5-C6-O6
2	J	769	NAG	C3-C2-N2-C7
3	I	1	JNH	O1-C5-N1-C4
3	I	1	JNH	C6-C5-N1-C4

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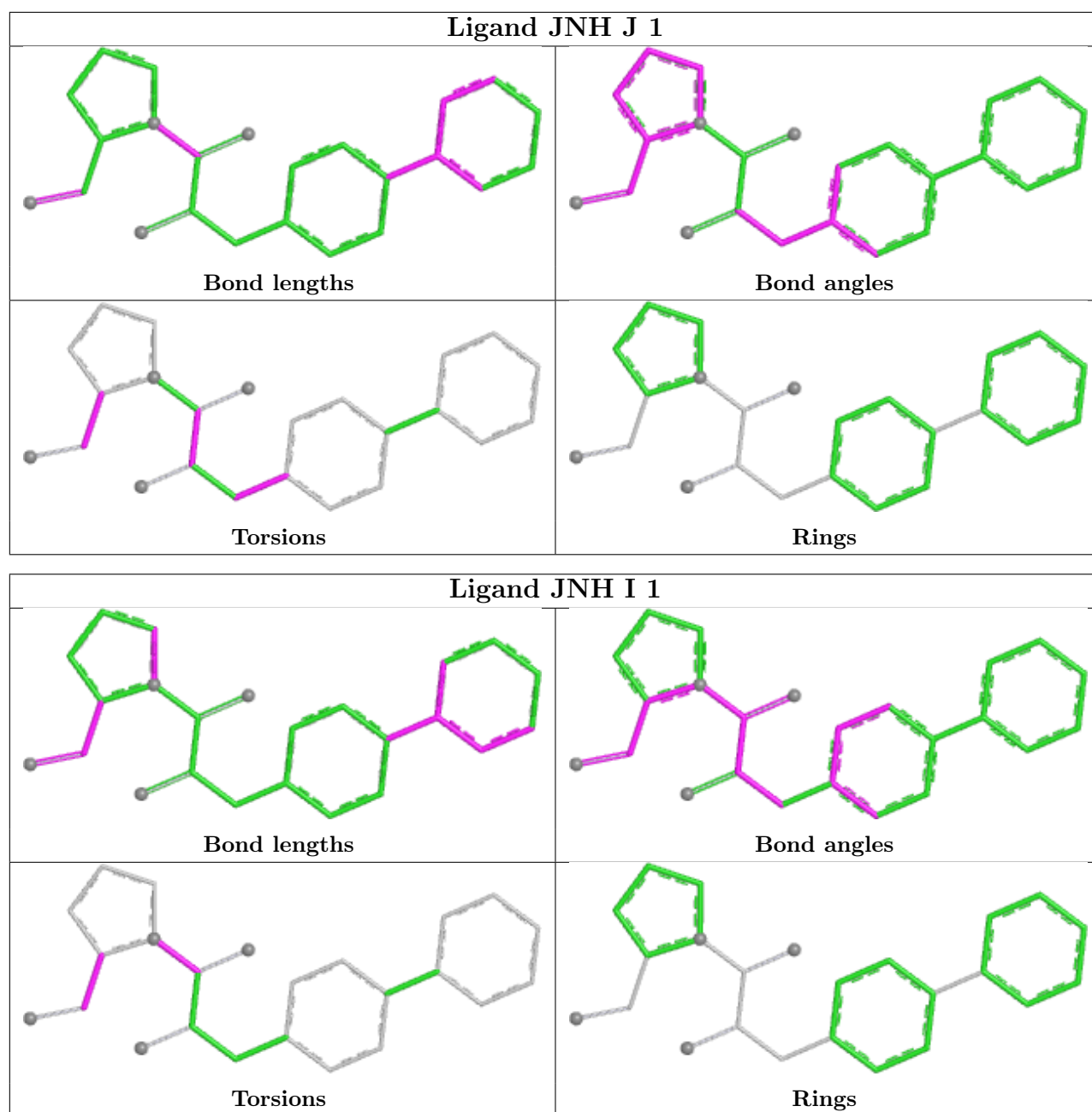
Mol	Chain	Res	Type	Atoms
3	J	1	JNH	O1-C5-C6-N2
2	I	771	NAG	C3-C2-N2-C7
3	J	1	JNH	N1-C5-C6-N2
2	I	771	NAG	C4-C5-C6-O6
2	I	771	NAG	C1-C2-N2-C7
2	J	768	NAG	C1-C2-N2-C7
2	J	769	NAG	C1-C2-N2-C7
2	J	774	NAG	C8-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	770	NAG	1	0
2	J	769	NAG	3	0
2	I	768	NAG	5	0
2	J	768	NAG	1	0
2	J	774	NAG	5	0
2	J	773	NAG	1	0
2	J	771	NAG	6	0
3	J	1	JNH	7	0
3	I	1	JNH	8	0
2	J	767	NAG	7	0
2	I	767	NAG	2	0
2	J	770	NAG	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	I	726/728 (99%)	0.82	74 (10%) 12 10	3, 19, 50, 80	0
1	J	728/728 (100%)	0.75	78 (10%) 11 9	3, 16, 49, 86	0
All	All	1454/1456 (99%)	0.78	152 (10%) 11 10	3, 18, 49, 86	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	98	PHE	6.7
1	I	95	PHE	6.4
1	I	99	GLY	5.8
1	J	94	THR	5.6
1	I	142	LEU	5.2
1	I	100	HIS	5.0
1	J	138	ASN	4.9
1	I	135	TYR	4.8
1	J	96	ASP	4.8
1	J	98	PHE	4.8
1	I	96	ASP	4.7
1	J	87	SER	4.6
1	I	102	ILE	4.6
1	J	72	GLN	4.4
1	I	101	SER	4.4
1	I	103	ASN	4.4
1	I	280	THR	4.3
1	J	92	ASN	4.3
1	J	86	SER	4.3
1	J	278	SER	4.3
1	I	279	VAL	4.2
1	J	389	ILE	4.1
1	J	103	ASN	4.1
1	J	95	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	66	HIS	4.0
1	I	114	ILE	4.0
1	J	141	GLN	3.9
1	I	147	ARG	3.9
1	J	93	SER	3.8
1	J	88	VAL	3.8
1	I	94	THR	3.6
1	J	279	VAL	3.6
1	I	276	LEU	3.6
1	J	508	GLN	3.6
1	J	100	HIS	3.6
1	J	137	LEU	3.6
1	J	40	ARG	3.5
1	I	487	ASN	3.5
1	J	73	GLU	3.5
1	I	113	PHE	3.5
1	I	73	GLU	3.4
1	I	277	SER	3.4
1	J	277	SER	3.4
1	I	149	PRO	3.2
1	J	97	GLU	3.2
1	I	93	SER	3.2
1	I	110	ASP	3.1
1	J	102	ILE	3.1
1	J	275	SER	3.1
1	I	151	ASN	3.1
1	I	138	ASN	3.1
1	I	140	ARG	3.1
1	J	143	ILE	3.1
1	I	180	LEU	3.0
1	J	142	LEU	3.0
1	J	506	ASN	3.0
1	I	333	SER	3.0
1	J	413	ASP	2.9
1	I	275	SER	2.9
1	I	143	ILE	2.9
1	I	148	ILE	2.9
1	J	144	THR	2.9
1	I	182	SER	2.9
1	J	74	ASN	2.9
1	I	65	ASP	2.8
1	J	766	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	505	GLN	2.8
1	J	75	ASN	2.8
1	I	141	GLN	2.7
1	J	388	GLN	2.7
1	J	85	ASN	2.7
1	J	391	LYS	2.7
1	I	130	ALA	2.7
1	J	488	ASP	2.6
1	I	278	SER	2.6
1	I	282	ALA	2.6
1	I	766	PRO	2.6
1	I	115	LEU	2.6
1	I	229	ASN	2.6
1	J	41	LYS	2.6
1	J	105	TYR	2.6
1	J	187	TRP	2.5
1	J	99	GLY	2.5
1	I	231	THR	2.5
1	J	183	TYR	2.5
1	I	132	TYR	2.5
1	I	522	THR	2.5
1	I	111	GLY	2.5
1	J	63	ILE	2.5
1	J	276	LEU	2.5
1	J	366	LEU	2.5
1	I	157	TRP	2.5
1	J	109	PRO	2.4
1	J	45	LEU	2.4
1	I	150	ASN	2.4
1	I	377	ASN	2.4
1	I	161	GLY	2.4
1	I	71	LYS	2.4
1	I	368	GLY	2.4
1	I	69	LEU	2.4
1	J	180	LEU	2.4
1	I	105	TYR	2.4
1	J	84	GLY	2.4
1	I	518	ILE	2.4
1	J	489	LYS	2.4
1	I	176	ILE	2.3
1	J	60	LEU	2.3
1	J	168	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	537	SER	2.3
1	J	90	LEU	2.3
1	J	139	LYS	2.3
1	J	507	VAL	2.3
1	I	308	GLN	2.3
1	J	101	SER	2.3
1	I	97	GLU	2.3
1	I	289	ALA	2.2
1	J	280	THR	2.2
1	I	761	GLN	2.2
1	J	71	LYS	2.2
1	J	487	ASN	2.2
1	I	168	TRP	2.2
1	I	89	PHE	2.2
1	I	160	VAL	2.2
1	J	160	VAL	2.2
1	I	74	ASN	2.2
1	I	121	VAL	2.2
1	I	511	SER	2.2
1	J	108	SER	2.2
1	I	187	TRP	2.2
1	J	157	TRP	2.2
1	J	534	PHE	2.2
1	I	144	THR	2.1
1	J	91	GLU	2.1
1	I	680	LEU	2.1
1	J	401	THR	2.1
1	I	134	ILE	2.1
1	J	367	ASP	2.1
1	J	478	PRO	2.1
1	J	219	ASN	2.1
1	I	296	GLY	2.1
1	J	70	TYR	2.1
1	I	697	GLN	2.1
1	J	289	ALA	2.1
1	I	189	GLY	2.1
1	J	466	LYS	2.1
1	J	66	HIS	2.1
1	J	390	ASP	2.0
1	I	284	SER	2.0
1	J	340	LEU	2.0
1	J	490	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	76	ILE	2.0
1	I	330	TYR	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](#)

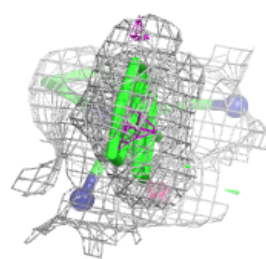
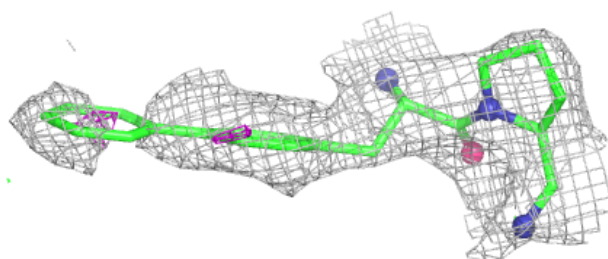
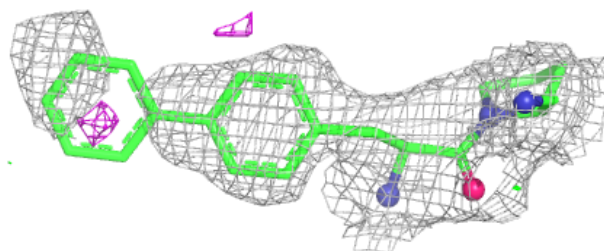
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	I	769	14/15	0.57	0.24	59,61,65,66	0
2	NAG	I	771	14/15	0.57	0.30	78,82,86,86	0
2	NAG	J	770	14/15	0.57	0.25	56,62,69,70	0
2	NAG	J	768	14/15	0.61	0.24	67,70,72,72	0
2	NAG	J	772	14/15	0.64	0.24	56,60,65,65	0
2	NAG	J	773	14/15	0.65	0.18	31,38,41,45	0
2	NAG	I	767	14/15	0.67	0.20	38,40,42,43	0
2	NAG	J	775	14/15	0.67	0.19	48,57,60,64	0
2	NAG	I	770	14/15	0.68	0.32	77,80,81,82	0
2	NAG	J	767	14/15	0.72	0.20	39,46,49,50	0
2	NAG	J	774	14/15	0.73	0.15	35,38,41,42	0
2	NAG	J	769	14/15	0.74	0.21	45,50,53,55	0
2	NAG	J	771	14/15	0.78	0.16	18,21,30,31	0
2	NAG	I	768	14/15	0.80	0.19	35,40,42,43	0
3	JNH	I	1	24/24	0.80	0.18	27,32,38,41	0
3	JNH	J	1	24/24	0.85	0.15	19,24,30,30	0

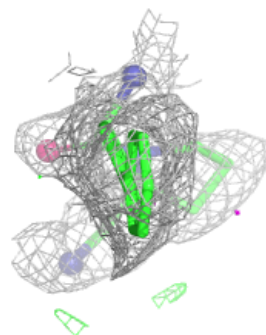
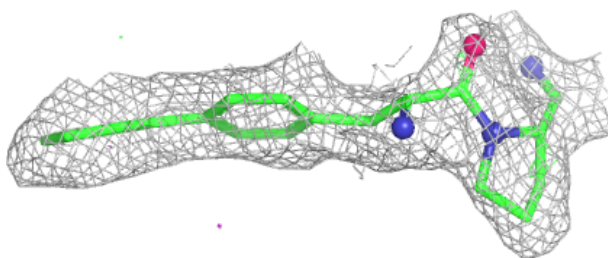
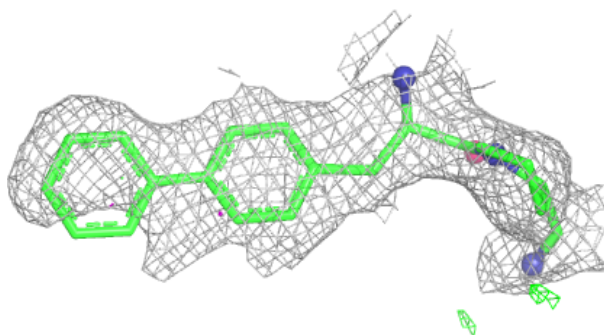
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JNH I 1:

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

**Electron density around JNH J 1:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.