



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:05 PM EDT

PDB ID : 4RBN / pdb_00004rbn
Title : The crystal structure of Nitrosomonas europaea sucrose synthase: Insights into the evolutionary origin of sucrose metabolism in prokaryotes
Authors : Wu, R.; Asencion Diez, M.D.; Figueroa, C.M.; Machtey, M.; Iglesias, A.A.; Ballicora, M.A.; Liu, D.
Deposited on : 2014-09-12
Resolution : 3.05 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

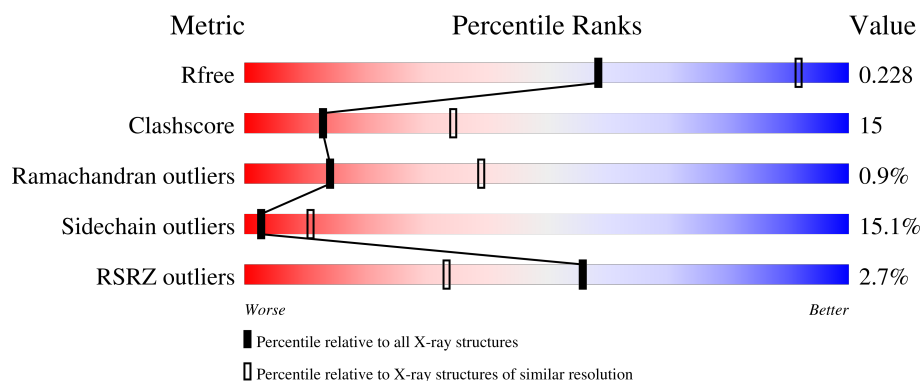
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	794	 2% 62% 30% 6% ..
1	B	794	 2% 61% 30% 8% ..
1	C	794	 2% 62% 29% 7% ..
1	D	794	 5% 54% 36% 9% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25595 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 Sucrose synthase:Glycosyl transferases group 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	789	Total	C	N	O	S	0	0	0
			6332	4033	1106	1165	28			
1	C	789	Total	C	N	O	S	0	0	0
			6360	4047	1112	1173	28			
1	B	789	Total	C	N	O	S	0	0	0
			6346	4040	1106	1172	28			
1	D	789	Total	C	N	O	S	0	0	0
			6352	4039	1111	1174	28			

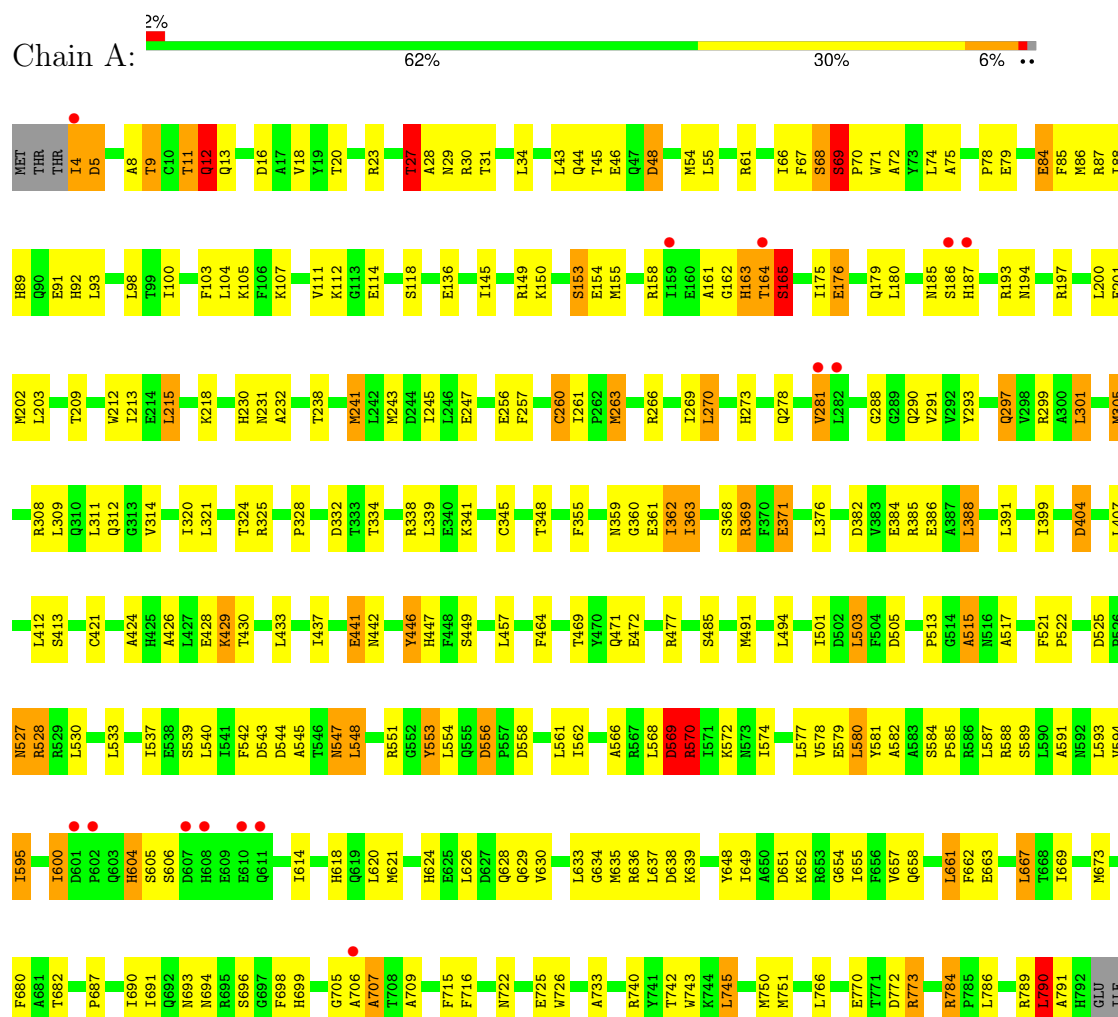
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	52	Total	O	0	0
			52	52		
2	C	50	Total	O	0	0
			50	50		
2	B	66	Total	O	0	0
			66	66		
2	D	37	Total	O	0	0
			37	37		

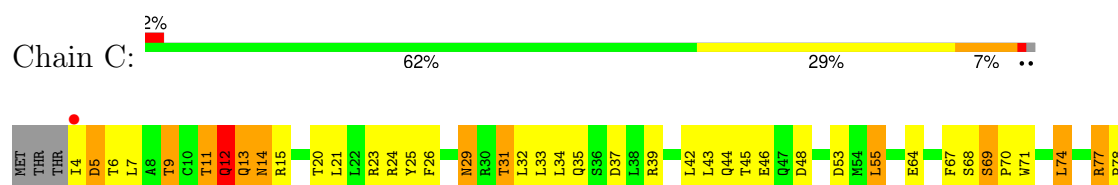
3 Residue-property plots [i](#)

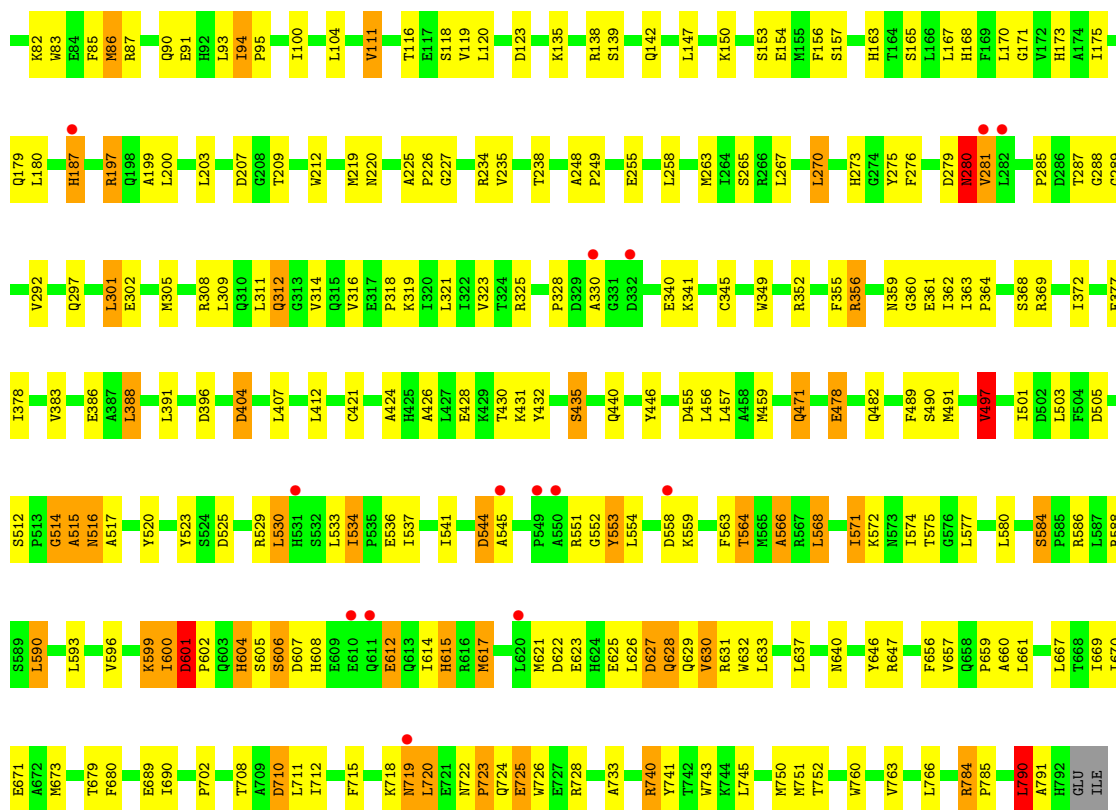
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sucrose synthase:Glycosyl transferases group 1

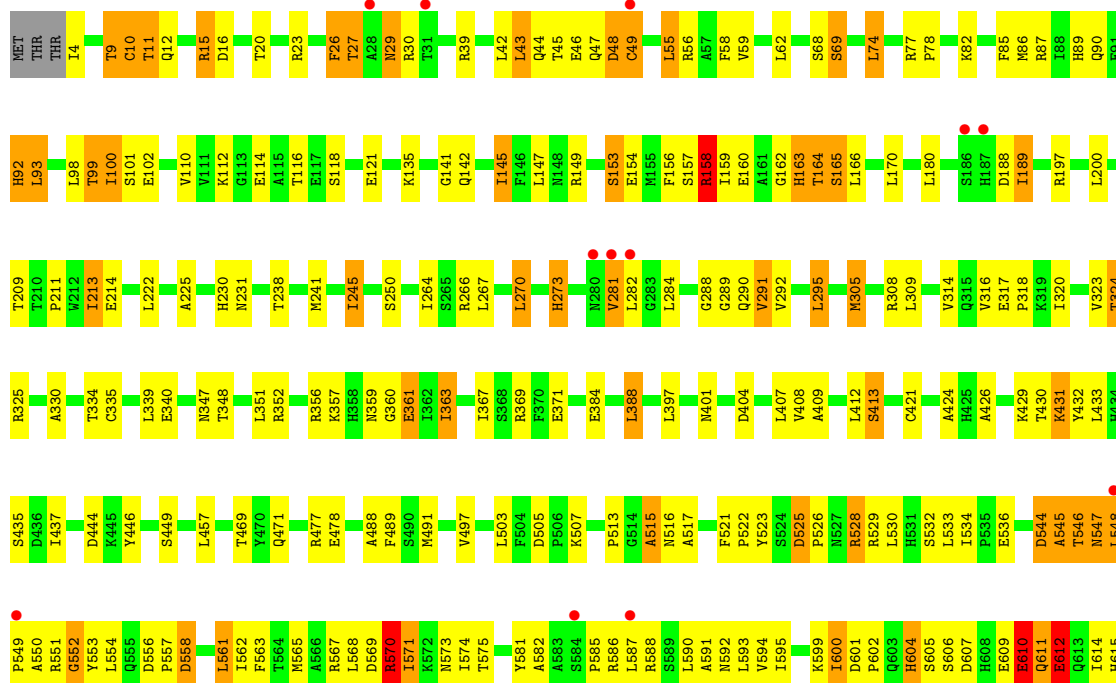


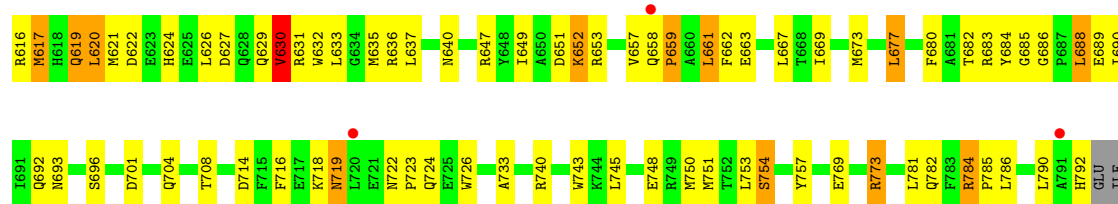
• Molecule 1: Sucrose synthase:Glycosyl transferases group 1



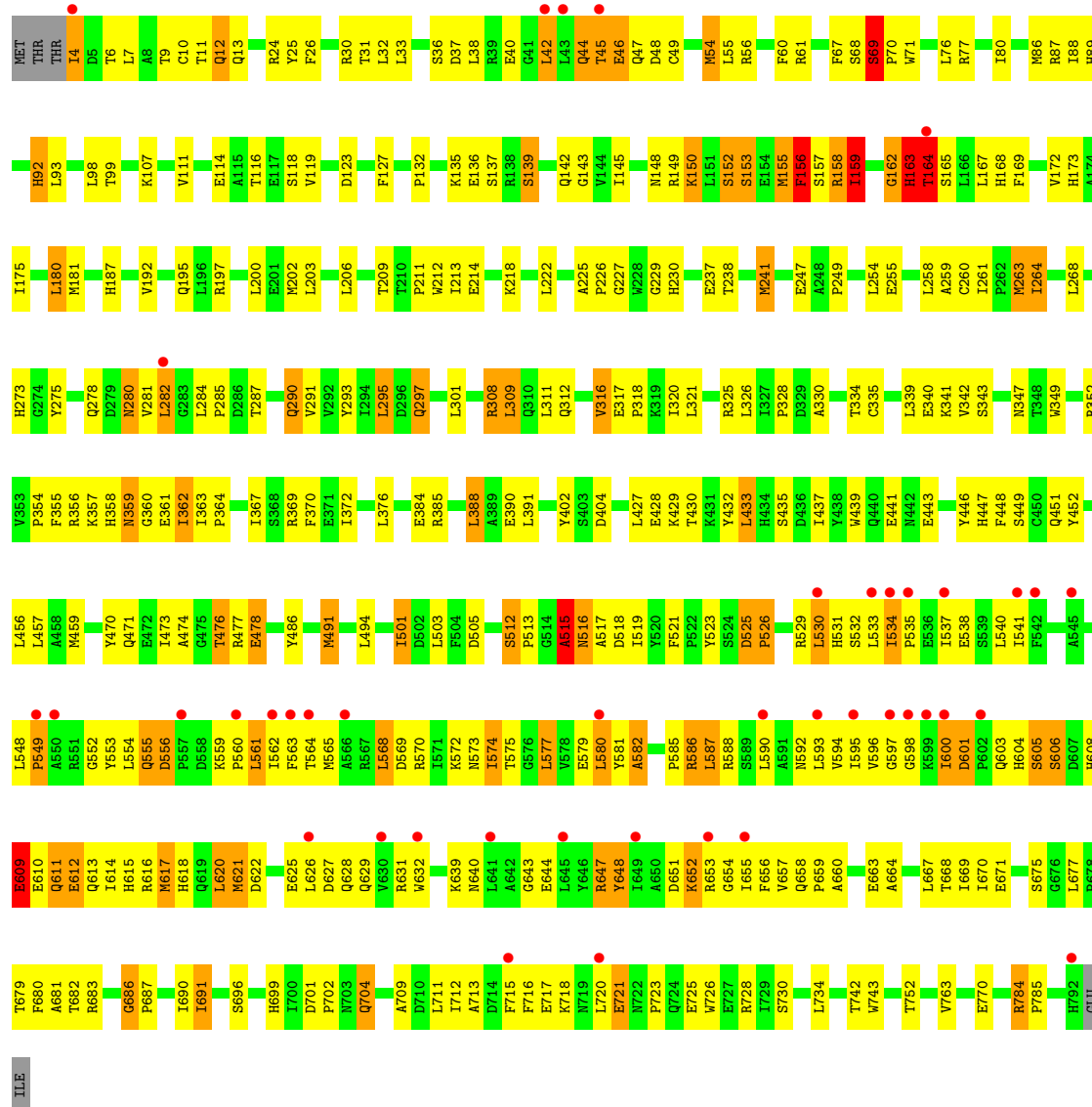


• Molecule 1: Sucrose synthase:Glycosyl transferases group 1





● Molecule 1: Sucrose synthase:Glycosyl transferases group 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	236.90Å 236.90Å 213.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.39 – 3.05 68.39 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (68.39-3.05) 93.5 (68.39-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.176 , 0.228 0.179 , 0.228	Depositor DCC
R_{free} test set	6337 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25595	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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

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	0.65	0/6481	1.12	32/8786 (0.4%)
1	B	0.61	0/6496	1.09	43/8806 (0.5%)
1	C	0.61	0/6511	1.07	37/8825 (0.4%)
1	D	0.60	0/6501	1.09	39/8812 (0.4%)
All	All	0.62	0/25989	1.09	151/35229 (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	A	0	6
1	B	0	5
1	C	0	6
1	D	0	12
All	All	0	29

There are no bond length outliers.

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	THR	N-CA-C	-14.12	96.06	113.28
1	D	164	THR	N-CA-C	-13.92	96.30	113.28
1	A	790	LEU	N-CA-C	12.04	128.19	113.38
1	D	704	GLN	N-CA-C	10.07	123.62	109.31
1	C	790	LEU	N-CA-C	9.35	125.14	111.96
1	D	362	ILE	N-CA-C	9.27	125.24	111.89
1	A	363	ILE	CA-C-N	8.92	128.57	118.85
1	A	363	ILE	C-N-CA	8.92	128.57	118.85
1	B	29	ASN	N-CA-C	-8.89	100.21	112.12
1	A	505	ASP	CA-C-N	-8.74	108.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	ASP	C-N-CA	-8.74	108.91	119.84
1	A	569	ASP	CA-C-N	8.70	137.35	121.70
1	A	569	ASP	C-N-CA	8.70	137.35	121.70
1	A	604	HIS	N-CA-C	8.41	121.28	111.02
1	A	446	TYR	N-CA-C	8.39	122.02	111.69
1	B	69	SER	CA-C-N	-8.34	110.64	121.91
1	B	69	SER	C-N-CA	-8.34	110.64	121.91
1	D	611	GLN	N-CA-C	-8.31	93.10	110.80
1	A	161	ALA	N-CA-C	-7.78	95.89	108.41
1	C	726	TRP	N-CA-C	-7.77	102.13	111.69
1	D	156	PHE	CA-C-N	7.75	135.65	121.70
1	D	156	PHE	C-N-CA	7.75	135.65	121.70
1	B	363	ILE	CA-C-N	7.72	127.00	118.97
1	B	363	ILE	C-N-CA	7.72	127.00	118.97
1	B	677	LEU	CA-C-N	7.57	128.00	119.83
1	B	677	LEU	C-N-CA	7.57	128.00	119.83
1	C	600	ILE	N-CA-C	7.55	119.16	108.36
1	A	545	ALA	N-CA-C	7.53	119.14	108.00
1	C	512	SER	CA-C-N	7.43	129.12	119.84
1	C	512	SER	C-N-CA	7.43	129.12	119.84
1	D	686	GLY	CA-C-N	-7.42	112.07	119.56
1	D	686	GLY	C-N-CA	-7.42	112.07	119.56
1	D	549	PRO	N-CA-C	7.34	122.34	111.03
1	D	586	ARG	N-CA-C	-7.29	104.36	113.18
1	B	601	ASP	CA-C-N	7.27	127.91	119.47
1	B	601	ASP	C-N-CA	7.27	127.91	119.47
1	B	158	ARG	N-CA-C	-7.25	103.52	112.88
1	B	546	THR	N-CA-C	7.11	122.83	113.30
1	C	584	SER	CA-C-N	7.02	126.84	119.05
1	C	584	SER	C-N-CA	7.02	126.84	119.05
1	B	612	GLU	N-CA-C	-6.97	104.58	113.23
1	A	600	ILE	N-CA-C	-6.91	102.52	110.05
1	D	512	SER	CA-C-N	6.90	128.46	119.84
1	D	512	SER	C-N-CA	6.90	128.46	119.84
1	A	584	SER	CA-C-N	6.89	126.49	119.19
1	A	584	SER	C-N-CA	6.89	126.49	119.19
1	A	158	ARG	N-CA-C	-6.86	104.52	113.17
1	A	740	ARG	N-CA-C	6.75	121.68	113.38
1	A	707	ALA	N-CA-C	-6.69	103.80	112.23
1	D	77	ARG	CA-C-N	6.69	126.48	119.05
1	D	77	ARG	C-N-CA	6.69	126.48	119.05
1	B	77	ARG	CA-C-N	6.64	126.42	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	C-N-CA	6.64	126.42	119.05
1	D	597	GLY	N-CA-C	6.59	118.21	111.95
1	C	77	ARG	CA-C-N	6.59	126.10	119.24
1	C	77	ARG	C-N-CA	6.59	126.10	119.24
1	D	516	ASN	CA-C-N	6.57	133.53	121.70
1	D	516	ASN	C-N-CA	6.57	133.53	121.70
1	C	544	ASP	N-CA-C	6.51	116.83	108.24
1	C	516	ASN	CA-C-N	6.50	133.40	121.70
1	C	516	ASN	C-N-CA	6.50	133.40	121.70
1	D	163	HIS	N-CA-C	-6.48	92.86	111.00
1	D	573	ASN	N-CA-C	6.38	120.04	111.24
1	D	552	GLY	N-CA-C	6.37	121.13	110.56
1	C	515	ALA	N-CA-C	6.36	117.98	108.31
1	C	505	ASP	CA-C-N	6.30	126.00	119.82
1	C	505	ASP	C-N-CA	6.30	126.00	119.82
1	D	627	ASP	N-CA-C	-6.28	105.49	113.02
1	B	156	PHE	CA-C-N	-6.25	113.60	122.41
1	B	156	PHE	C-N-CA	-6.25	113.60	122.41
1	D	7	LEU	N-CA-C	-6.23	105.16	112.89
1	B	528	ARG	N-CA-C	6.23	120.48	113.01
1	C	163	HIS	N-CA-C	6.22	118.91	109.95
1	B	27	THR	N-CA-C	-6.22	100.98	110.30
1	D	143	GLY	N-CA-C	6.19	120.13	112.64
1	B	658	GLN	CA-C-N	6.14	127.52	119.84
1	B	658	GLN	C-N-CA	6.14	127.52	119.84
1	D	12	GLN	N-CA-C	-6.12	105.85	113.38
1	A	165	SER	N-CA-C	-6.01	104.42	110.97
1	C	330	ALA	N-CA-C	-5.99	104.66	111.07
1	C	446	TYR	N-CA-C	5.95	119.01	111.69
1	D	505	ASP	CA-C-N	5.92	125.62	119.82
1	D	505	ASP	C-N-CA	5.92	125.62	119.82
1	A	68	SER	N-CA-C	-5.91	98.67	108.07
1	A	542	PHE	N-CA-C	5.91	120.62	113.17
1	C	491	MET	CA-C-N	5.91	125.93	119.90
1	C	491	MET	C-N-CA	5.91	125.93	119.90
1	B	637	LEU	CB-CA-C	-5.84	108.84	115.79
1	C	281	VAL	N-CA-C	5.83	118.61	112.83
1	D	162	GLY	CA-C-O	-5.76	118.30	122.45
1	C	515	ALA	CB-CA-C	-5.76	109.92	116.54
1	B	558	ASP	N-CA-C	-5.75	106.27	113.28
1	A	591	ALA	N-CA-C	5.73	115.80	108.24
1	B	225	ALA	CA-C-N	-5.71	114.88	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ALA	C-N-CA	-5.71	114.88	120.98
1	B	719	ASN	N-CA-C	5.70	117.58	110.91
1	D	347	ASN	N-CA-C	5.69	119.92	112.92
1	C	566	ALA	N-CA-C	5.67	115.72	108.24
1	A	790	LEU	CA-C-N	5.66	131.88	121.70
1	A	790	LEU	C-N-CA	5.66	131.88	121.70
1	D	515	ALA	N-CA-C	-5.63	98.80	110.80
1	B	446	TYR	N-CA-C	5.63	119.32	112.23
1	D	71	TRP	N-CA-C	5.60	119.37	109.96
1	C	607	ASP	N-CA-C	5.59	117.45	110.91
1	D	363	ILE	CA-C-N	5.59	125.20	119.56
1	D	363	ILE	C-N-CA	5.59	125.20	119.56
1	C	545	ALA	CB-CA-C	-5.49	110.26	116.63
1	D	525	ASP	N-CA-C	5.47	117.44	109.30
1	B	165	SER	N-CA-C	-5.44	106.31	113.17
1	B	505	ASP	CA-C-N	5.44	125.15	119.82
1	B	505	ASP	C-N-CA	5.44	125.15	119.82
1	B	264	ILE	N-CA-C	5.44	115.42	107.37
1	D	664	ALA	N-CA-C	5.43	117.63	111.11
1	A	5	ASP	N-CA-C	5.43	115.53	107.88
1	A	260	CYS	CB-CA-C	-5.42	101.64	110.85
1	C	723	PRO	CA-C-N	5.42	131.45	121.70
1	C	723	PRO	C-N-CA	5.42	131.45	121.70
1	A	69	SER	CA-C-N	-5.41	113.07	119.84
1	A	69	SER	C-N-CA	-5.41	113.07	119.84
1	C	497	VAL	CB-CA-C	-5.33	102.89	110.83
1	A	545	ALA	CB-CA-C	-5.33	108.88	116.34
1	B	515	ALA	CA-C-N	5.32	131.27	121.70
1	B	515	ALA	C-N-CA	5.32	131.27	121.70
1	C	5	ASP	N-CA-C	5.30	115.36	107.88
1	B	145	ILE	CB-CA-C	-5.29	105.20	111.81
1	B	266	ARG	N-CA-C	5.28	117.33	107.99
1	D	391	LEU	N-CA-C	-5.28	103.56	110.53
1	C	12	GLN	CA-C-N	5.24	131.80	122.31
1	C	12	GLN	C-N-CA	5.24	131.80	122.31
1	D	622	ASP	N-CA-C	5.23	118.97	112.58
1	A	27	THR	N-CA-C	-5.22	100.58	108.67
1	B	769	GLU	N-CA-C	5.18	117.60	111.33
1	C	545	ALA	N-CA-C	5.18	116.83	108.08
1	D	264	ILE	N-CA-C	5.16	114.17	106.85
1	B	548	LEU	N-CA-C	-5.11	102.60	110.32
1	C	171	GLY	N-CA-C	5.11	119.94	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	719	ASN	N-CA-C	5.11	117.21	108.67
1	C	111	VAL	N-CA-C	5.10	115.31	110.42
1	B	544	ASP	N-CA-C	5.09	121.65	110.80
1	B	141	GLY	CA-C-N	-5.09	114.99	123.33
1	B	141	GLY	C-N-CA	-5.09	114.99	123.33
1	D	376	LEU	N-CA-C	5.07	116.89	111.36
1	B	112	LYS	N-CA-C	5.06	119.15	112.92
1	B	604	HIS	CA-C-N	5.06	130.82	121.70
1	B	604	HIS	C-N-CA	5.06	130.82	121.70
1	C	790	LEU	CA-C-N	5.06	130.81	121.70
1	C	790	LEU	C-N-CA	5.06	130.81	121.70
1	A	515	ALA	CA-C-N	5.04	130.77	121.70
1	A	515	ALA	C-N-CA	5.04	130.77	121.70
1	B	630	VAL	N-CA-C	5.03	115.22	108.17
1	D	165	SER	N-CA-C	-5.03	105.07	111.11

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLN	Peptide
1	A	13	GLN	Peptide
1	A	27	THR	Peptide
1	A	359	ASN	Peptide
1	A	551	ARG	Peptide
1	A	569	ASP	Peptide
1	B	163	HIS	Peptide
1	B	359	ASN	Peptide
1	B	545	ALA	Peptide
1	B	552	GLY	Peptide
1	B	570	ARG	Peptide
1	C	13	GLN	Peptide
1	C	359	ASN	Peptide
1	C	514	GLY	Peptide
1	C	599	LYS	Peptide
1	C	720	LEU	Peptide
1	C	790	LEU	Peptide
1	D	13	GLN	Peptide
1	D	155	MET	Peptide
1	D	159	ILE	Peptide
1	D	359	ASN	Peptide
1	D	526	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	D	548	LEU	Peptide
1	D	549	PRO	Peptide
1	D	563	PHE	Peptide
1	D	582	ALA	Peptide
1	D	606	SER	Peptide
1	D	609	GLU	Peptide
1	D	702	PRO	Peptide

5.2 Too-close contacts [i](#)

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	6332	0	6210	174	0
1	B	6346	0	6220	189	0
1	C	6360	0	6240	176	0
1	D	6352	0	6235	229	0
2	A	52	0	0	1	0
2	B	66	0	0	4	0
2	C	50	0	0	0	0
2	D	37	0	0	0	0
All	All	25595	0	24905	753	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 15.

All (753) 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:D:516:ASN:HB3	1:D:518:ASP:H	1.25	1.01
1:D:654:GLY:O	1:D:655:ILE:HD13	1.66	0.94
1:D:360:GLY:HA2	1:D:361:GLU:HB3	1.52	0.91
1:D:654:GLY:O	1:D:655:ILE:CD1	2.22	0.86
1:D:369:ARG:NH2	1:D:428:GLU:OE2	2.08	0.86
1:B:604:HIS:HB2	1:B:605:SER:HB3	1.58	0.86
1:A:515:ALA:HB3	1:A:743:TRP:HD1	1.42	0.83
1:D:157:SER:O	1:D:159:ILE:N	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ALA:HB3	1:B:743:TRP:HD1	1.43	0.81
1:D:716:PHE:HA	1:D:721:GLU:HG3	1.62	0.80
1:A:162:GLY:HA2	1:A:164:THR:H	1.45	0.80
1:D:579:GLU:HG2	1:D:580:LEU:HD22	1.65	0.79
1:A:657:VAL:HG22	1:A:680:PHE:HB2	1.64	0.78
1:A:669:ILE:HG22	1:A:673:MET:HE2	1.63	0.78
1:D:611:GLN:O	1:D:614:ILE:N	2.15	0.78
1:B:288:GLY:H	1:B:290:GLN:HG3	1.48	0.78
1:A:136:GLU:OE2	1:C:197:ARG:NH1	2.16	0.78
1:D:340:GLU:OE1	1:D:352:ARG:NH2	2.16	0.77
1:C:12:GLN:HA	1:C:15:ARG:HB3	1.65	0.77
1:B:340:GLU:OE1	1:B:352:ARG:NH2	2.16	0.77
1:D:162:GLY:HA2	1:D:164:THR:H	1.50	0.76
1:C:340:GLU:OE1	1:C:352:ARG:NH2	2.18	0.76
1:D:4:ILE:HG21	1:D:61:ARG:HG3	1.69	0.75
1:C:718:LYS:O	1:C:722:ASN:N	2.19	0.75
1:B:586:ARG:NH2	1:B:714:ASP:OD2	2.19	0.75
1:D:281:VAL:HG13	1:D:284:LEU:HD12	1.69	0.74
1:A:43:LEU:HA	1:A:46:GLU:HB2	1.69	0.74
1:D:54:MET:HG2	1:D:55:LEU:HD23	1.68	0.74
1:D:644:GLU:HA	1:D:648:TYR:HE1	1.51	0.74
1:B:360:GLY:HA2	1:B:361:GLU:HB2	1.69	0.73
1:C:123:ASP:OD2	1:B:773:ARG:NH1	2.21	0.73
1:B:515:ALA:HB3	1:B:743:TRP:CD1	2.24	0.72
1:B:356:ARG:HB3	1:B:360:GLY:HA3	1.70	0.72
1:B:669:ILE:HG22	1:B:673:MET:HE2	1.72	0.71
1:C:69:SER:HB2	1:C:70:PRO:HD2	1.72	0.71
1:D:577:LEU:HB2	1:D:659:PRO:HG3	1.70	0.71
1:D:616:ARG:HH11	1:D:620:LEU:HD21	1.55	0.71
1:C:621:MET:HE3	1:C:630:VAL:HG22	1.73	0.71
1:A:706:ALA:HA	1:A:709:ALA:HB3	1.73	0.70
1:C:715:PHE:O	1:C:722:ASN:ND2	2.23	0.70
1:B:549:PRO:HB3	1:B:600:ILE:HB	1.73	0.70
1:C:287:THR:HG22	1:C:288:GLY:H	1.56	0.70
1:B:682:THR:HG22	1:B:684:TYR:H	1.54	0.70
1:D:521:PHE:HB2	1:D:647:ARG:HH11	1.57	0.70
1:C:571:ILE:HA	1:C:661:LEU:HD12	1.74	0.70
1:C:33:LEU:HB2	1:C:67:PHE:HE2	1.57	0.70
1:A:360:GLY:HA2	1:A:361:GLU:HB3	1.73	0.69
1:D:357:LYS:O	1:D:359:ASN:N	2.25	0.68
1:D:530:LEU:HB2	1:D:648:TYR:CE2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:ILE:HG22	1:D:564:THR:HG23	1.73	0.68
1:B:4:ILE:HD11	1:B:58:PHE:HA	1.75	0.68
1:D:604:HIS:HA	1:D:606:SER:N	2.09	0.68
1:C:305:MET:HE3	1:C:318:PRO:HB2	1.74	0.68
1:A:162:GLY:HA2	1:A:164:THR:N	2.09	0.68
1:D:157:SER:C	1:D:159:ILE:H	2.00	0.68
1:D:554:LEU:O	1:D:559:LYS:NZ	2.28	0.67
1:C:369:ARG:NH2	1:C:428:GLU:OE2	2.28	0.67
1:D:155:MET:HA	1:D:157:SER:HB2	1.76	0.67
1:C:360:GLY:HA2	1:C:361:GLU:HB2	1.77	0.67
1:B:43:LEU:HA	1:B:46:GLU:HB2	1.75	0.67
1:C:588:ARG:HH11	1:C:629:GLN:HG3	1.60	0.67
1:C:622:ASP:OD2	1:C:623:GLU:N	2.27	0.66
1:B:528:ARG:HG3	1:B:528:ARG:HH11	1.60	0.66
1:C:11:THR:C	1:C:13:GLN:H	2.03	0.66
1:C:719:ASN:ND2	1:C:724:GLN:OE1	2.29	0.66
1:D:515:ALA:HB1	1:D:516:ASN:HA	1.75	0.66
1:A:582:ALA:HA	1:A:588:ARG:HE	1.60	0.66
1:D:654:GLY:O	1:D:655:ILE:CG1	2.43	0.66
1:D:515:ALA:HB3	1:D:743:TRP:HD1	1.60	0.66
1:B:250:SER:HB3	1:D:149:ARG:HD3	1.78	0.66
1:C:173:HIS:CE1	1:C:263:MET:HE3	2.30	0.66
1:B:163:HIS:N	1:B:164:THR:O	2.29	0.66
1:A:118:SER:O	1:D:784:ARG:NH2	2.27	0.66
1:B:701:ASP:HB3	1:B:704:GLN:HB2	1.76	0.66
1:D:644:GLU:HA	1:D:648:TYR:CE1	2.31	0.65
1:C:275:TYR:HE1	1:C:285:PRO:HG2	1.62	0.65
1:D:574:ILE:H	1:D:574:ILE:HD12	1.61	0.65
1:A:784:ARG:NH2	1:D:118:SER:O	2.25	0.65
1:D:449:SER:HA	1:D:491:MET:HE3	1.77	0.65
1:D:643:GLY:O	1:D:647:ARG:NH2	2.27	0.65
1:B:610:GLU:C	1:B:612:GLU:H	2.04	0.65
1:A:569:ASP:HB2	1:A:570:ARG:HB3	1.79	0.64
1:A:673:MET:HG2	1:A:733:ALA:HB1	1.80	0.64
1:D:24:ARG:HH21	1:D:44:GLN:HB3	1.61	0.64
1:D:281:VAL:HG11	1:D:287:THR:HG21	1.79	0.64
1:D:516:ASN:HA	1:D:517:ALA:HB3	1.79	0.64
1:D:651:ASP:N	1:D:652:LYS:O	2.31	0.64
1:D:162:GLY:HA2	1:D:164:THR:N	2.12	0.64
1:D:600:ILE:HD12	1:D:617:MET:HE1	1.78	0.64
1:C:29:ASN:OD1	1:C:29:ASN:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:626:LEU:HB3	1:D:628:GLN:H	1.64	0.63
1:A:580:LEU:HD12	1:A:709:ALA:HB2	1.79	0.63
1:B:621:MET:HA	1:B:626:LEU:HD12	1.81	0.63
1:A:48:ASP:N	1:A:48:ASP:OD1	2.32	0.63
1:A:469:THR:OG1	1:A:472:GLU:HG3	1.98	0.63
1:A:649:ILE:HG22	1:A:654:GLY:HA3	1.80	0.62
1:D:452:TYR:HB2	1:D:491:MET:HE1	1.81	0.62
1:C:523:TYR:HA	1:C:647:ARG:HG2	1.80	0.62
1:D:155:MET:HB2	1:D:249:PRO:HG3	1.82	0.62
1:B:673:MET:HG2	1:B:733:ALA:HB1	1.81	0.62
1:D:404:ASP:OD1	1:D:404:ASP:N	2.31	0.62
1:D:587:LEU:HG	1:D:709:ALA:HB2	1.81	0.61
1:D:717:GLU:HG3	1:D:718:LYS:H	1.64	0.61
1:C:600:ILE:HG23	1:C:601:ASP:O	2.01	0.61
1:B:158:ARG:NH2	1:B:159:ILE:HG12	2.15	0.61
1:D:357:LYS:C	1:D:359:ASN:H	2.06	0.61
1:D:553:TYR:N	1:D:628:GLN:O	2.30	0.61
1:B:16:ASP:O	1:B:20:THR:OG1	2.12	0.61
1:B:48:ASP:OD1	1:B:48:ASP:N	2.31	0.61
1:B:26:PHE:CE2	1:B:90:GLN:HB2	2.36	0.60
1:A:515:ALA:HB1	1:A:517:ALA:N	2.17	0.60
1:C:600:ILE:HG21	1:C:614:ILE:HG23	1.84	0.60
1:A:61:ARG:HD3	1:A:78:PRO:HA	1.83	0.60
1:A:162:GLY:H	1:A:164:THR:HG23	1.66	0.60
1:A:515:ALA:HB3	1:A:743:TRP:CD1	2.31	0.60
1:B:135:LYS:HB2	1:D:247:GLU:HG3	1.83	0.60
1:B:521:PHE:HB2	1:B:522:PRO:HD2	1.83	0.60
1:D:720:LEU:HD13	1:D:723:PRO:HG2	1.84	0.60
1:D:654:GLY:O	1:D:655:ILE:HG12	2.02	0.60
1:D:175:ILE:HG12	1:D:180:LEU:HD22	1.84	0.59
1:D:515:ALA:HB3	1:D:743:TRP:CD1	2.37	0.59
1:B:360:GLY:HA2	1:B:361:GLU:CB	2.30	0.59
1:D:459:MET:HE3	1:D:501:ILE:HB	1.84	0.59
1:C:723:PRO:HD2	1:C:724:GLN:HB2	1.83	0.59
1:C:784:ARG:NH2	1:B:118:SER:O	2.33	0.59
1:A:382:ASP:OD1	1:A:385:ARG:NH1	2.31	0.59
1:A:421:CYS:SG	1:A:750:MET:HE1	2.43	0.59
1:A:163:HIS:ND1	1:A:165:SER:HB2	2.17	0.59
1:B:568:LEU:HD12	1:B:574:ILE:HD13	1.85	0.59
1:B:523:TYR:O	1:B:529:ARG:HD2	2.03	0.59
1:C:428:GLU:HG2	1:C:431:LYS:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:PHE:HE2	1:B:90:GLN:HB2	1.68	0.58
1:A:269:ILE:HD12	1:A:399:ILE:HD12	1.85	0.58
1:D:167:LEU:HD13	1:D:192:VAL:HG21	1.86	0.58
1:B:431:LYS:HE2	1:B:432:TYR:CZ	2.37	0.58
1:C:584:SER:O	1:C:588:ARG:HG3	2.03	0.58
1:B:477:ARG:HH11	1:B:477:ARG:HB3	1.69	0.58
1:B:85:PHE:CE2	1:B:100:ILE:HG12	2.38	0.58
1:D:562:ILE:HG22	1:D:564:THR:CG2	2.32	0.58
1:A:9:THR:O	1:A:12:GLN:HG3	2.03	0.58
1:B:790:LEU:C	1:B:792:HIS:H	2.10	0.58
1:D:238:THR:HA	1:D:241:MET:HE3	1.86	0.58
1:C:604:HIS:HA	1:C:605:SER:C	2.28	0.58
1:A:693:ASN:HB2	1:A:699:HIS:ND1	2.19	0.57
1:D:656:PHE:HB2	1:D:677:LEU:HD23	1.86	0.57
1:B:324:THR:OG1	1:B:325:ARG:N	2.35	0.57
1:B:547:ASN:OD1	1:B:547:ASN:N	2.32	0.57
1:B:599:LYS:HB2	1:B:614:ILE:HD11	1.86	0.57
1:B:652:LYS:HG2	1:B:653:ARG:HG2	1.86	0.57
1:A:150:LYS:NZ	1:A:154:GLU:OE1	2.37	0.57
1:C:227:GLY:O	1:C:312:GLN:HG3	2.04	0.57
1:D:570:ARG:HD3	1:D:610:GLU:HG2	1.85	0.57
1:D:621:MET:HB2	1:D:632:TRP:CH2	2.39	0.57
1:C:669:ILE:HG23	1:C:679:THR:HG21	1.86	0.57
1:C:670:ILE:HD11	1:C:690:ILE:HD13	1.87	0.57
1:B:550:ALA:HB1	1:B:551:ARG:HA	1.87	0.57
1:C:360:GLY:HA2	1:C:361:GLU:CB	2.33	0.57
1:C:328:PRO:HG2	1:C:364:PRO:HA	1.85	0.57
1:A:270:LEU:HD21	1:A:412:LEU:HD12	1.87	0.57
1:C:627:ASP:OD1	1:C:627:ASP:N	2.29	0.57
1:B:44:GLN:N	1:B:46:GLU:H	2.03	0.57
1:B:273:HIS:C	1:B:273:HIS:CD2	2.83	0.57
1:A:572:LYS:NZ	1:A:663:GLU:OE1	2.36	0.56
1:C:632:TRP:HD1	1:C:633:LEU:N	2.03	0.56
1:A:441:GLU:OE1	1:A:441:GLU:N	2.38	0.56
1:C:356:ARG:HB3	1:C:360:GLY:HA3	1.86	0.56
1:A:569:ASP:HB2	1:A:570:ARG:HD2	1.85	0.56
1:C:150:LYS:NZ	1:C:154:GLU:OE1	2.37	0.56
1:D:341:LYS:HB2	1:D:349:TRP:CZ3	2.41	0.56
1:A:355:PHE:HB3	1:A:363:ILE:HD12	1.87	0.56
1:B:15:ARG:HH11	1:B:15:ARG:HB3	1.69	0.56
1:D:92:HIS:CD2	1:D:92:HIS:H	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LEU:HA	1:A:580:LEU:HD23	1.88	0.56
1:B:320:ILE:HB	1:B:348:THR:HG23	1.86	0.56
1:B:288:GLY:N	1:B:290:GLN:HG3	2.19	0.56
1:B:657:VAL:HG22	1:B:680:PHE:HB2	1.88	0.56
1:A:562:ILE:HD11	1:A:716:PHE:HE2	1.71	0.56
1:A:773:ARG:NH1	1:D:123:ASP:OD2	2.39	0.55
1:C:459:MET:CE	1:C:501:ILE:HB	2.36	0.55
1:B:609:GLU:O	1:B:611:GLN:NE2	2.38	0.55
1:A:87:ARG:HB3	1:A:98:LEU:HD11	1.87	0.55
1:C:600:ILE:HG12	1:C:614:ILE:HG13	1.87	0.55
1:A:79:GLU:OE2	1:A:477:ARG:NH2	2.39	0.55
1:A:111:VAL:HG12	1:A:112:LYS:HG2	1.88	0.55
1:A:369:ARG:NH2	1:A:428:GLU:OE1	2.39	0.55
1:A:566:ALA:HB3	1:A:574:ILE:HD11	1.89	0.55
1:D:582:ALA:HA	1:D:585:PRO:HG3	1.88	0.55
1:D:660:ALA:HB3	1:D:663:GLU:HB2	1.87	0.55
1:D:211:PRO:HB2	1:D:213:ILE:HG22	1.87	0.55
1:D:325:ARG:HH12	1:D:367:ILE:HG13	1.71	0.55
1:B:544:ASP:HB3	1:B:553:TYR:CD1	2.41	0.55
1:B:723:PRO:HG2	1:B:724:GLN:NE2	2.22	0.55
1:A:230:HIS:CG	1:A:231:ASN:H	2.24	0.55
1:C:42:LEU:HD11	1:C:55:LEU:HD12	1.89	0.55
1:C:43:LEU:HA	1:C:46:GLU:HB2	1.89	0.55
1:B:424:ALA:C	1:B:426:ALA:H	2.15	0.55
1:C:24:ARG:HG3	1:C:45:THR:HG23	1.89	0.55
1:D:601:ASP:OD2	1:D:605:SER:OG	2.25	0.55
1:D:668:THR:HA	1:D:671:GLU:OE2	2.07	0.55
1:A:368:SER:HB3	1:A:371:GLU:HG3	1.88	0.54
1:B:267:LEU:HD22	1:B:305:MET:HE2	1.88	0.54
1:D:433:LEU:H	1:D:433:LEU:HD22	1.72	0.54
1:A:238:THR:HG21	1:A:312:GLN:HE22	1.72	0.54
1:A:297:GLN:HG3	1:A:301:LEU:HD22	1.90	0.54
1:C:725:GLU:OE2	1:C:728:ARG:NH1	2.39	0.54
1:B:289:GLY:O	1:B:292:VAL:HG12	2.08	0.54
1:B:357:LYS:HG3	1:B:363:ILE:HD11	1.89	0.54
1:D:326:LEU:HD13	1:D:354:PRO:HG3	1.89	0.54
1:A:149:ARG:O	1:A:153:SER:HB3	2.08	0.54
1:C:219:MET:HE3	1:C:235:VAL:HG11	1.89	0.54
1:D:593:LEU:HD22	1:D:595:ILE:HD11	1.90	0.54
1:A:288:GLY:C	1:A:290:GLN:H	2.14	0.54
1:A:593:LEU:HD13	1:A:595:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:NH1	1:D:136:GLU:OE2	2.41	0.54
1:B:633:LEU:HD22	1:B:635:MET:HE1	1.90	0.54
1:A:11:THR:HG23	1:A:54:MET:HE3	1.90	0.54
1:B:305:MET:HG2	1:B:751:MET:SD	2.48	0.54
1:C:369:ARG:HH22	1:C:428:GLU:CD	2.15	0.54
1:D:175:ILE:HG21	1:D:316:VAL:HG21	1.89	0.54
1:A:23:ARG:O	1:A:27:THR:HG23	2.07	0.53
1:D:11:THR:OG1	1:D:55:LEU:HD21	2.08	0.53
1:D:360:GLY:HA2	1:D:361:GLU:CB	2.23	0.53
1:C:723:PRO:CD	1:C:724:GLN:HB2	2.37	0.53
1:B:397:LEU:HD22	1:B:754:SER:HB3	1.90	0.53
1:A:164:THR:HB	1:A:187:HIS:CD2	2.44	0.53
1:A:547:ASN:OD1	1:A:547:ASN:N	2.41	0.53
1:B:449:SER:HA	1:B:491:MET:HE1	1.90	0.53
1:B:574:ILE:HD12	1:B:574:ILE:H	1.73	0.53
1:A:513:PRO:HB3	1:A:743:TRP:CZ2	2.43	0.53
1:C:784:ARG:HB3	1:C:785:PRO:HD3	1.90	0.53
1:D:111:VAL:HG21	1:D:437:ILE:HG12	1.91	0.53
1:D:617:MET:HG2	1:D:632:TRP:HZ2	1.73	0.53
1:A:28:ALA:C	1:A:30:ARG:H	2.15	0.53
1:A:540:LEU:HB3	1:A:633:LEU:HD21	1.89	0.53
1:B:211:PRO:HG2	1:B:214:GLU:HG2	1.91	0.53
1:D:297:GLN:HB2	1:D:743:TRP:CZ3	2.43	0.53
1:D:565:MET:HG3	1:D:596:VAL:HB	1.90	0.53
1:D:568:LEU:HD22	1:D:598:GLY:HA3	1.90	0.53
1:D:569:ASP:HB3	1:D:572:LYS:HB2	1.90	0.53
1:A:163:HIS:CG	1:A:165:SER:HB2	2.44	0.53
1:B:42:LEU:HD13	1:B:59:VAL:HG21	1.90	0.53
1:B:602:PRO:HD3	1:B:614:ILE:HG21	1.91	0.53
1:B:611:GLN:N	2:B:846:HOH:O	2.42	0.53
1:D:6:THR:O	1:D:9:THR:HG22	2.09	0.52
1:B:554:LEU:HD12	1:B:554:LEU:H	1.75	0.52
1:D:617:MET:SD	1:D:632:TRP:NE1	2.82	0.52
1:B:291:VAL:HG13	1:B:295:LEU:HD23	1.90	0.52
1:D:604:HIS:NE2	1:D:612:GLU:HG3	2.25	0.52
1:C:6:THR:HG23	1:C:7:LEU:HD12	1.90	0.52
1:A:324:THR:OG1	1:A:325:ARG:N	2.42	0.52
1:D:669:ILE:HG23	1:D:679:THR:HG21	1.91	0.52
1:A:299:ARG:HG2	1:A:345:CYS:SG	2.49	0.52
1:A:582:ALA:HB1	1:A:624:HIS:ND1	2.25	0.52
1:C:566:ALA:HB1	1:C:572:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASP:N	1:A:556:ASP:OD2	2.43	0.52
1:B:10:CYS:C	1:B:12:GLN:H	2.17	0.52
1:C:9:THR:C	1:C:11:THR:H	2.17	0.52
1:C:156:PHE:CD2	1:C:249:PRO:HD2	2.45	0.52
1:D:139:SER:O	1:D:142:GLN:HB2	2.10	0.52
1:D:291:VAL:O	1:D:295:LEU:HB2	2.10	0.52
1:C:20:THR:HG23	1:C:23:ARG:HH21	1.75	0.51
1:B:421:CYS:SG	1:B:750:MET:HE1	2.50	0.51
1:C:552:GLY:HA3	1:C:631:ARG:HA	1.92	0.51
1:C:599:LYS:O	1:C:601:ASP:HB2	2.09	0.51
1:D:691:ILE:HG22	1:D:699:HIS:NE2	2.25	0.51
1:A:569:ASP:HB2	1:A:570:ARG:CD	2.40	0.51
1:B:42:LEU:HD21	1:B:56:ARG:HG2	1.93	0.51
1:D:603:GLN:H	1:D:603:GLN:NE2	2.09	0.51
1:A:600:ILE:H	1:A:634:GLY:HA3	1.75	0.51
1:B:571:ILE:HD11	1:B:662:PHE:H	1.76	0.51
1:D:679:THR:HG22	1:D:681:ALA:H	1.76	0.51
1:C:459:MET:HE1	1:C:501:ILE:HB	1.93	0.51
1:C:516:ASN:HA	1:C:517:ALA:HB3	1.92	0.51
1:D:132:PRO:HG3	1:D:150:LYS:HD2	1.91	0.51
1:D:608:HIS:ND1	1:D:611:GLN:HG2	2.25	0.51
1:C:424:ALA:C	1:C:426:ALA:H	2.18	0.51
1:C:514:GLY:O	1:C:743:TRP:NE1	2.44	0.51
1:D:473:ILE:HG22	1:D:503:LEU:HD12	1.93	0.51
1:D:92:HIS:H	1:D:92:HIS:HD2	1.58	0.51
1:A:155:MET:HG3	1:A:163:HIS:HB2	1.93	0.50
1:A:288:GLY:H	1:A:290:GLN:HG3	1.74	0.50
1:A:338:ARG:HH21	1:A:386:GLU:HG2	1.76	0.50
1:B:647:ARG:NH1	2:B:839:HOH:O	2.43	0.50
1:D:541:ILE:O	1:D:631:ARG:NH1	2.25	0.50
1:C:612:GLU:O	1:C:615:HIS:HB2	2.12	0.50
1:D:87:ARG:HB3	1:D:98:LEU:HD11	1.93	0.50
1:A:31:THR:HB	1:A:67:PHE:O	2.11	0.50
1:A:528:ARG:HH11	1:A:528:ARG:CG	2.23	0.50
1:C:657:VAL:HG22	1:C:680:PHE:HB2	1.93	0.50
1:D:173:HIS:CE1	1:D:263:MET:HE3	2.46	0.50
1:A:593:LEU:HD22	1:A:595:ILE:HD11	1.93	0.50
1:C:6:THR:HA	1:C:86:MET:HE1	1.93	0.50
1:D:521:PHE:O	1:D:675:SER:HA	2.10	0.50
1:A:85:PHE:CZ	1:A:100:ILE:HD13	2.46	0.50
1:A:569:ASP:CA	1:A:570:ARG:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LEU:HD13	1:D:598:GLY:HA3	1.92	0.50
1:D:784:ARG:HB3	1:D:785:PRO:HD3	1.93	0.50
1:C:377:GLU:OE1	1:C:784:ARG:NH1	2.44	0.50
1:B:89:HIS:HB3	1:B:92:HIS:O	2.12	0.50
1:D:355:PHE:O	1:D:356:ARG:HG3	2.12	0.50
1:D:370:PHE:CE1	1:D:446:TYR:HD1	2.30	0.50
1:D:526:PRO:HA	1:D:529:ARG:HB2	1.93	0.50
1:B:600:ILE:HG12	1:B:632:TRP:CH2	2.47	0.50
1:D:157:SER:O	1:D:159:ILE:HG13	2.11	0.50
1:C:270:LEU:HD21	1:C:412:LEU:HD12	1.94	0.50
1:D:227:GLY:O	1:D:312:GLN:HB3	2.11	0.50
1:D:586:ARG:HH11	1:D:713:ALA:HB2	1.76	0.50
1:A:527:ASN:OD1	1:A:527:ASN:N	2.45	0.50
1:A:587:LEU:HD22	1:A:709:ALA:HB1	1.94	0.50
1:A:384:GLU:O	1:A:388:LEU:HB2	2.12	0.49
1:C:421:CYS:SG	1:C:750:MET:HE1	2.52	0.49
1:B:158:ARG:HB2	1:B:162:GLY:HA3	1.94	0.49
1:D:156:PHE:H	1:D:158:ARG:HB3	1.76	0.49
1:A:633:LEU:HD23	1:A:635:MET:SD	2.52	0.49
1:B:288:GLY:C	1:B:290:GLN:H	2.20	0.49
1:D:155:MET:HE3	1:D:254:LEU:HD21	1.94	0.49
1:D:470:TYR:CE1	1:D:474:ALA:HB3	2.47	0.49
1:D:562:ILE:CG2	1:D:564:THR:CG2	2.90	0.49
1:C:621:MET:HG3	1:C:626:LEU:HD12	1.94	0.49
1:B:92:HIS:H	1:B:92:HIS:CD2	2.30	0.49
1:B:429:LYS:HE2	1:B:489:PHE:CG	2.47	0.49
1:B:575:THR:HA	1:B:617:MET:HE1	1.95	0.49
1:B:582:ALA:HB1	1:B:624:HIS:CE1	2.48	0.49
1:A:442:ASN:HB3	1:A:446:TYR:HD2	1.76	0.49
1:A:722:ASN:CG	1:A:726:TRP:H	2.19	0.49
1:C:77:ARG:HD2	1:C:83:TRP:CZ2	2.48	0.49
1:C:673:MET:HB3	1:C:733:ALA:HB1	1.94	0.49
1:B:515:ALA:HB1	1:B:516:ASN:HA	1.94	0.49
1:B:563:PHE:CZ	1:B:565:MET:HE2	2.48	0.49
1:D:30:ARG:NH2	1:D:37:ASP:OD2	2.45	0.49
1:C:33:LEU:HD22	1:C:37:ASP:HB2	1.95	0.49
1:C:596:VAL:HG11	1:C:637:LEU:HG	1.95	0.49
1:D:600:ILE:HG13	1:D:618:HIS:CE1	2.47	0.49
1:C:328:PRO:HD2	1:C:364:PRO:O	2.13	0.49
1:D:212:TRP:CZ2	1:D:226:PRO:HA	2.48	0.49
1:D:491:MET:O	1:D:494:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:HA	1:A:231:ASN:HB2	1.93	0.49
1:A:621:MET:HA	1:A:626:LEU:CG	2.43	0.49
1:C:118:SER:O	1:B:784:ARG:NH2	2.29	0.49
1:B:10:CYS:C	1:B:12:GLN:N	2.71	0.49
1:B:588:ARG:HH11	1:B:629:GLN:HE21	1.60	0.49
1:B:784:ARG:HB3	1:B:785:PRO:HD3	1.95	0.49
1:B:153:SER:HA	1:D:153:SER:HB2	1.95	0.49
1:B:568:LEU:HA	1:B:574:ILE:HD13	1.95	0.49
1:A:569:ASP:HA	1:A:570:ARG:HB3	1.95	0.48
1:C:33:LEU:HB2	1:C:67:PHE:CE2	2.44	0.48
1:D:42:LEU:HD11	1:D:56:ARG:HH11	1.77	0.48
1:D:617:MET:HG2	1:D:632:TRP:CZ2	2.48	0.48
1:A:569:ASP:CB	1:A:570:ARG:HB3	2.42	0.48
1:C:614:ILE:HA	1:C:617:MET:HB2	1.95	0.48
1:B:101:SER:OG	1:B:121:GLU:OE2	2.31	0.48
1:D:581:TYR:CE1	1:D:587:LEU:HB3	2.48	0.48
1:B:163:HIS:O	1:B:166:LEU:HB3	2.13	0.48
1:B:570:ARG:HA	2:B:851:HOH:O	2.13	0.48
1:D:476:THR:HB	1:D:478:GLU:OE2	2.13	0.48
1:D:701:ASP:O	1:D:704:GLN:HB2	2.13	0.48
1:A:4:ILE:HG23	1:A:8:ALA:HB2	1.94	0.48
1:B:325:ARG:HH12	1:B:367:ILE:HG13	1.77	0.48
1:B:563:PHE:HZ	1:B:565:MET:HE2	1.78	0.48
1:D:428:GLU:HG3	1:D:451:GLN:OE1	2.14	0.48
1:C:577:LEU:HD12	1:C:580:LEU:HD11	1.96	0.48
1:D:609:GLU:O	1:D:609:GLU:HG3	2.13	0.48
1:D:670:ILE:HD11	1:D:690:ILE:HD13	1.96	0.48
1:A:449:SER:HA	1:A:491:MET:HE1	1.94	0.48
1:B:59:VAL:HA	1:B:62:LEU:HD12	1.95	0.48
1:B:611:GLN:O	1:B:615:HIS:ND1	2.46	0.48
1:D:321:LEU:HD11	1:D:390:GLU:HB3	1.95	0.48
1:D:330:ALA:HB2	1:D:335:CYS:HB2	1.94	0.48
1:C:203:LEU:HD21	1:C:219:MET:HE2	1.95	0.48
1:A:578:VAL:O	1:A:581:TYR:HB3	2.14	0.48
1:A:626:LEU:O	1:A:630:VAL:HB	2.14	0.48
1:A:673:MET:HE1	1:A:690:ILE:HG22	1.95	0.48
1:D:654:GLY:C	1:D:655:ILE:HG12	2.38	0.48
1:D:156:PHE:H	1:D:158:ARG:CB	2.27	0.47
1:D:308:ARG:NH2	1:D:752:THR:OG1	2.46	0.47
1:D:429:LYS:HG3	1:D:452:TYR:CE2	2.48	0.47
1:A:89:HIS:CE1	1:A:91:GLU:H	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:GLN:O	1:D:559:LYS:HB2	2.14	0.47
1:A:694:ASN:HA	1:A:698:PHE:CE1	2.50	0.47
1:C:529:ARG:HE	1:C:529:ARG:HB3	1.52	0.47
1:A:8:ALA:O	1:A:11:THR:OG1	2.31	0.47
1:A:212:TRP:N	1:A:230:HIS:O	2.47	0.47
1:A:328:PRO:HG3	1:A:362:ILE:HD11	1.95	0.47
1:A:722:ASN:HD21	1:A:725:GLU:HG2	1.79	0.47
1:D:647:ARG:H	1:D:647:ARG:HG2	1.34	0.47
1:A:539:SER:O	1:A:543:ASP:HB2	2.13	0.47
1:D:275:TYR:HD1	1:D:335:CYS:SG	2.38	0.47
1:A:558:ASP:N	1:A:558:ASP:OD2	2.47	0.47
1:A:680:PHE:CD2	1:A:698:PHE:HB2	2.49	0.47
1:C:276:PHE:O	1:C:281:VAL:HG11	2.14	0.47
1:B:471:GLN:HG3	1:B:689:GLU:OE1	2.14	0.47
1:B:515:ALA:HB1	1:B:517:ALA:N	2.29	0.47
1:D:259:ALA:HB2	1:D:752:THR:HG23	1.97	0.47
1:D:264:ILE:O	1:D:309:LEU:HD21	2.15	0.47
1:D:428:GLU:HB3	1:D:432:TYR:CE2	2.50	0.47
1:D:639:LYS:H	1:D:639:LYS:HD2	1.79	0.47
1:A:320:ILE:HB	1:A:348:THR:HG23	1.97	0.47
1:C:355:PHE:C	1:C:356:ARG:HG2	2.39	0.47
1:C:533:LEU:O	1:C:537:ILE:HG13	2.14	0.47
1:C:623:GLU:C	1:C:625:GLU:H	2.21	0.47
1:D:155:MET:HB3	1:D:158:ARG:NH1	2.30	0.47
1:D:592:ASN:O	1:D:593:LEU:HG	2.15	0.47
1:C:234:ARG:O	1:C:238:THR:HG23	2.15	0.47
1:D:195:GLN:NE2	1:D:222:LEU:O	2.34	0.47
1:D:293:TYR:O	1:D:297:GLN:HB3	2.15	0.47
1:D:427:LEU:HD13	1:D:486:TYR:CE1	2.50	0.47
1:C:85:PHE:CZ	1:C:100:ILE:HD13	2.50	0.47
1:C:302:GLU:OE1	1:C:345:CYS:HB3	2.15	0.47
1:D:169:PHE:O	1:D:172:VAL:HG22	2.15	0.47
1:D:586:ARG:HH11	1:D:713:ALA:CB	2.28	0.47
1:C:515:ALA:HB1	1:C:517:ALA:HB2	1.97	0.46
1:C:751:MET:HE2	1:C:751:MET:HA	1.97	0.46
1:B:318:PRO:O	1:B:347:ASN:HB3	2.16	0.46
1:B:325:ARG:NH1	1:B:367:ILE:HG13	2.31	0.46
1:D:568:LEU:HA	1:D:574:ILE:HD13	1.96	0.46
1:D:617:MET:HE3	1:D:632:TRP:CZ2	2.50	0.46
1:D:691:ILE:HG22	1:D:699:HIS:HE2	1.80	0.46
1:D:284:LEU:HB3	1:D:285:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:GLU:HB3	1:D:432:TYR:HE2	1.81	0.46
1:A:568:LEU:HD12	1:A:574:ILE:HD13	1.98	0.46
1:B:610:GLU:C	1:B:612:GLU:N	2.73	0.46
1:D:148:ASN:O	1:D:152:SER:HB3	2.14	0.46
1:A:66:ILE:HD11	1:A:107:LYS:HD2	1.96	0.46
1:A:562:ILE:HG12	1:A:655:ILE:HG12	1.98	0.46
1:C:790:LEU:H	1:C:791:ALA:HB3	1.79	0.46
1:B:270:LEU:O	1:B:401:ASN:HB2	2.16	0.46
1:B:550:ALA:O	1:B:600:ILE:HG21	2.16	0.46
1:B:653:ARG:HA	1:B:726:TRP:CE2	2.51	0.46
1:C:120:LEU:HD22	1:B:781:LEU:HD21	1.97	0.46
1:B:15:ARG:HB3	1:B:15:ARG:NH1	2.31	0.46
1:B:561:LEU:HD11	1:B:594:VAL:HG23	1.97	0.46
1:C:74:LEU:HB2	1:C:86:MET:HG2	1.97	0.46
1:C:355:PHE:HZ	1:C:372:ILE:HD11	1.80	0.46
1:C:719:ASN:HB3	1:C:723:PRO:HD2	1.97	0.46
1:B:554:LEU:HD23	1:B:592:ASN:CG	2.40	0.46
1:D:432:TYR:HB2	1:D:435:SER:OG	2.16	0.46
1:A:770:GLU:HG2	1:D:127:PHE:CD2	2.51	0.46
1:C:459:MET:HE2	1:C:459:MET:HB2	1.75	0.46
1:B:593:LEU:HB3	1:B:630:VAL:HG12	1.97	0.46
1:B:692:GLN:H	1:B:696:SER:HB2	1.81	0.46
1:A:585:PRO:HG2	2:A:843:HOH:O	2.15	0.46
1:C:601:ASP:HB3	1:C:602:PRO:HD2	1.98	0.46
1:B:78:PRO:HD2	1:B:82:LYS:O	2.15	0.46
1:D:107:LYS:HG2	1:D:437:ILE:HD13	1.98	0.46
1:D:158:ARG:HH11	1:D:163:HIS:HB2	1.80	0.46
1:D:211:PRO:HG2	1:D:214:GLU:HG3	1.97	0.46
1:D:290:GLN:HB2	1:D:402:TYR:OH	2.16	0.46
1:D:604:HIS:CD2	1:D:606:SER:HB2	2.50	0.46
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.63	0.46
1:A:288:GLY:C	1:A:290:GLN:N	2.73	0.46
1:A:540:LEU:HB3	1:A:633:LEU:CD2	2.45	0.46
1:C:690:ILE:HA	1:C:741:TYR:OH	2.15	0.46
1:B:44:GLN:N	1:B:46:GLU:N	2.64	0.46
1:B:330:ALA:HB2	1:B:335:CYS:HB2	1.97	0.46
1:A:618:HIS:O	1:A:621:MET:HB3	2.16	0.45
1:D:512:SER:HA	1:D:513:PRO:HD3	1.61	0.45
1:B:515:ALA:HB1	1:B:516:ASN:CA	2.46	0.45
1:D:683:ARG:HB2	1:D:683:ARG:CZ	2.46	0.45
1:A:247:GLU:HG3	1:C:135:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:HH11	1:A:528:ARG:HB2	1.82	0.45
1:B:87:ARG:HB3	1:B:98:LEU:HD11	1.99	0.45
1:B:99:THR:OG1	1:B:102:GLU:HG3	2.16	0.45
1:B:282:LEU:HD22	1:B:636:ARG:NH2	2.30	0.45
1:D:258:LEU:HD23	1:D:261:ILE:HD11	1.98	0.45
1:A:43:LEU:HD23	1:A:43:LEU:H	1.82	0.45
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.68	0.45
1:B:409:ALA:O	1:B:413:SER:HB3	2.16	0.45
1:B:615:HIS:O	1:B:619:GLN:HB2	2.16	0.45
1:B:616:ARG:O	1:B:620:LEU:HB2	2.17	0.45
1:D:680:PHE:CE2	1:D:711:LEU:HD21	2.50	0.45
1:B:48:ASP:HA	1:B:49:CYS:HA	1.50	0.45
1:B:323:VAL:HA	1:B:351:LEU:O	2.17	0.45
1:B:626:LEU:O	1:B:629:GLN:HB2	2.16	0.45
1:D:494:LEU:HD23	1:D:494:LEU:HA	1.71	0.45
1:D:555:GLN:CD	1:D:556:ASP:H	2.23	0.45
1:A:69:SER:HB3	1:A:70:PRO:HD2	1.99	0.45
1:C:520:TYR:CD2	1:C:671:GLU:HG2	2.52	0.45
1:A:72:ALA:HB3	1:A:88:ILE:HG22	1.98	0.45
1:A:193:ARG:O	1:A:197:ARG:HG3	2.17	0.45
1:C:566:ALA:HB3	1:C:574:ILE:HD11	1.97	0.45
1:C:605:SER:HA	1:C:606:SER:HA	1.36	0.45
1:C:632:TRP:CD1	1:C:632:TRP:C	2.93	0.45
1:A:261:ILE:HG22	1:A:263:MET:HG2	1.99	0.45
1:C:626:LEU:HB3	1:C:630:VAL:HG13	1.98	0.45
1:D:533:LEU:HB2	1:D:537:ILE:HG12	1.99	0.45
1:A:203:LEU:HD22	1:A:232:ALA:HB1	1.99	0.45
1:A:230:HIS:CD2	1:A:231:ASN:H	2.35	0.45
1:A:621:MET:HA	1:A:626:LEU:HG	1.99	0.45
1:C:11:THR:C	1:C:13:GLN:N	2.71	0.45
1:C:78:PRO:HD2	1:C:82:LYS:O	2.16	0.45
1:C:724:GLN:O	1:C:725:GLU:HB3	2.16	0.45
1:B:651:ASP:HA	1:B:652:LYS:HA	1.57	0.45
1:D:168:HIS:HB2	1:D:187:HIS:CE1	2.51	0.45
1:D:441:GLU:OE1	1:D:441:GLU:N	2.42	0.45
1:B:11:THR:HG21	1:B:55:LEU:HD23	1.98	0.45
1:A:449:SER:HA	1:A:491:MET:CE	2.47	0.44
1:A:651:ASP:HA	1:A:652:LYS:HA	1.70	0.44
1:C:568:LEU:HD22	1:C:568:LEU:HA	1.85	0.44
1:C:577:LEU:HB2	1:C:659:PRO:HG3	1.99	0.44
1:D:439:TRP:CD1	1:D:491:MET:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:PRO:HB2	1:D:588:ARG:H	1.82	0.44
1:A:153:SER:HB2	1:C:153:SER:HA	2.00	0.44
1:A:293:TYR:O	1:A:297:GLN:HB3	2.17	0.44
1:A:537:ILE:HG22	1:A:648:TYR:HD2	1.82	0.44
1:B:773:ARG:HA	1:B:773:ARG:HD3	1.86	0.44
1:A:257:PHE:O	1:A:260:CYS:HB2	2.17	0.44
1:C:33:LEU:HD23	1:C:33:LEU:HA	1.67	0.44
1:C:432:TYR:O	1:C:435:SER:OG	2.26	0.44
1:C:478:GLU:H	1:C:478:GLU:HG2	1.60	0.44
1:B:571:ILE:HD12	1:B:661:LEU:HB2	1.97	0.44
1:D:384:GLU:O	1:D:388:LEU:HB2	2.17	0.44
1:D:686:GLY:O	1:D:690:ILE:HG13	2.17	0.44
1:A:528:ARG:HH11	1:A:528:ARG:HG3	1.82	0.44
1:C:279:ASP:OD2	1:C:280:ASN:N	2.50	0.44
1:B:683:ARG:HE	1:B:684:TYR:HE1	1.65	0.44
1:D:26:PHE:CE1	1:D:67:PHE:HB3	2.52	0.44
1:D:278:GLN:C	1:D:280:ASN:H	2.26	0.44
1:B:291:VAL:HG13	1:B:295:LEU:CD2	2.48	0.44
1:B:605:SER:HA	1:B:606:SER:HA	1.71	0.44
1:A:569:ASP:HB2	1:A:570:ARG:CB	2.46	0.44
1:D:155:MET:O	1:D:156:PHE:HB2	2.18	0.44
1:D:523:TYR:O	1:D:526:PRO:HD3	2.17	0.44
1:B:12:GLN:O	1:B:15:ARG:HG3	2.18	0.44
1:D:328:PRO:HD2	1:D:364:PRO:HA	1.98	0.44
1:A:429:LYS:HE2	1:A:485:SER:OG	2.17	0.44
1:A:705:GLY:C	1:A:707:ALA:H	2.26	0.44
1:C:456:LEU:HD21	1:C:497:VAL:HG11	2.00	0.44
1:C:601:ASP:N	1:C:601:ASP:OD1	2.51	0.44
1:B:39:ARG:NH2	1:B:478:GLU:OE1	2.50	0.44
1:B:241:MET:O	1:B:245:ILE:HD12	2.17	0.44
1:B:281:VAL:HG11	1:B:291:VAL:HG11	1.99	0.44
1:D:46:GLU:HG3	1:D:47:GLN:HG3	2.00	0.44
1:D:570:ARG:H	1:D:570:ARG:HG2	1.63	0.44
1:C:9:THR:C	1:C:11:THR:N	2.75	0.44
1:C:199:ALA:O	1:C:203:LEU:HG	2.17	0.44
1:B:267:LEU:HB2	1:B:320:ILE:HG12	2.00	0.44
1:B:562:ILE:HD11	1:B:716:PHE:HE2	1.83	0.44
1:D:158:ARG:O	1:D:158:ARG:HG3	2.18	0.44
1:D:268:LEU:HD12	1:D:321:LEU:HB2	1.99	0.44
1:C:170:LEU:HA	1:C:170:LEU:HD23	1.74	0.43
1:B:551:ARG:HB2	1:B:552:GLY:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:TYR:OH	1:B:591:ALA:O	2.31	0.43
1:A:273:HIS:HD2	1:A:404:ASP:OD1	2.01	0.43
1:C:48:ASP:OD1	1:C:48:ASP:N	2.51	0.43
1:C:147:LEU:HD21	1:C:760:TRP:HB2	1.99	0.43
1:C:471:GLN:HG2	1:C:689:GLU:OE1	2.18	0.43
1:D:715:PHE:CD2	1:D:726:TRP:HB2	2.53	0.43
1:A:44:GLN:HA	1:A:45:THR:HA	1.80	0.43
1:B:513:PRO:HB3	1:B:743:TRP:CH2	2.53	0.43
1:B:513:PRO:HB3	1:B:743:TRP:CZ2	2.53	0.43
1:A:305:MET:HG2	1:A:751:MET:SD	2.57	0.43
1:C:147:LEU:HD11	1:C:760:TRP:CD2	2.54	0.43
1:B:188:ASP:O	1:B:189:ILE:HB	2.18	0.43
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.70	0.43
1:C:323:VAL:HG11	1:C:383:VAL:HG13	2.00	0.43
1:C:404:ASP:OD1	1:C:404:ASP:N	2.48	0.43
1:C:455:ASP:O	1:C:459:MET:HG3	2.17	0.43
1:B:281:VAL:HA	1:B:284:LEU:HD12	2.00	0.43
1:A:360:GLY:HA2	1:A:361:GLU:CB	2.40	0.43
1:C:31:THR:HG22	1:C:67:PHE:O	2.19	0.43
1:C:544:ASP:N	1:C:544:ASP:OD1	2.51	0.43
1:B:790:LEU:C	1:B:792:HIS:N	2.77	0.43
1:D:582:ALA:HA	1:D:585:PRO:CG	2.49	0.43
1:D:680:PHE:CZ	1:D:711:LEU:HD21	2.53	0.43
1:A:175:ILE:HG22	1:A:176:GLU:HG2	2.00	0.43
1:A:528:ARG:HH11	1:A:528:ARG:CB	2.32	0.43
1:C:71:TRP:CZ3	1:C:87:ARG:HD2	2.53	0.43
1:C:258:LEU:HD23	1:C:258:LEU:HA	1.75	0.43
1:C:297:GLN:HB2	1:C:743:TRP:CZ3	2.53	0.43
1:D:604:HIS:HA	1:D:606:SER:H	1.84	0.43
1:A:12:GLN:HB3	1:A:18:VAL:HG21	1.99	0.43
1:A:215:LEU:H	1:A:215:LEU:HG	1.69	0.43
1:C:26:PHE:CE2	1:C:90:GLN:HB2	2.54	0.43
1:D:212:TRP:N	1:D:230:HIS:O	2.50	0.43
1:D:669:ILE:HD13	1:D:687:PRO:HB3	2.00	0.43
1:C:281:VAL:HB	1:C:287:THR:HG21	2.00	0.43
1:C:600:ILE:HA	1:C:601:ASP:HB2	2.00	0.43
1:B:288:GLY:C	1:B:290:GLN:N	2.77	0.43
1:B:610:GLU:O	1:B:612:GLU:N	2.52	0.43
1:D:588:ARG:NH2	1:D:629:GLN:HG3	2.33	0.43
1:C:646:TYR:HE1	1:C:656:PHE:CE2	2.37	0.43
1:A:667:LEU:HD23	1:A:667:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ARG:HA	1:A:789:ARG:HD3	1.86	0.42
1:C:20:THR:HG23	1:C:23:ARG:NH2	2.34	0.42
1:C:94:ILE:HA	1:C:95:PRO:HD3	1.85	0.42
1:C:308:ARG:NH2	1:C:752:THR:OG1	2.52	0.42
1:B:384:GLU:O	1:B:388:LEU:HB2	2.19	0.42
1:D:44:GLN:HA	1:D:45:THR:HA	1.55	0.42
1:D:309:LEU:HD13	1:D:309:LEU:HA	1.83	0.42
1:D:429:LYS:HG3	1:D:452:TYR:CZ	2.53	0.42
1:D:429:LYS:HA	1:D:452:TYR:OH	2.19	0.42
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.77	0.42
1:A:433:LEU:HA	1:A:433:LEU:HD23	1.65	0.42
1:A:540:LEU:HD23	1:A:548:LEU:HD22	2.01	0.42
1:A:605:SER:N	1:A:606:SER:HA	2.34	0.42
1:B:620:LEU:HD22	1:B:620:LEU:HA	1.92	0.42
1:A:544:ASP:HB3	1:A:553:TYR:CD2	2.55	0.42
1:C:362:ILE:HD12	1:C:362:ILE:H	1.84	0.42
1:C:740:ARG:HB3	1:C:741:TYR:CD2	2.55	0.42
1:B:573:ASN:HB3	1:B:659:PRO:O	2.19	0.42
1:B:627:ASP:C	1:B:629:GLN:H	2.28	0.42
1:B:669:ILE:HG22	1:B:673:MET:CE	2.46	0.42
1:D:711:LEU:H	1:D:711:LEU:HD23	1.84	0.42
1:B:9:THR:C	1:B:11:THR:H	2.26	0.42
1:B:55:LEU:O	1:B:59:VAL:HG23	2.19	0.42
1:B:180:LEU:HA	1:B:180:LEU:HD23	1.81	0.42
1:D:585:PRO:HB3	1:D:587:LEU:HB2	2.01	0.42
1:C:552:GLY:H	1:C:631:ARG:HH11	1.67	0.42
1:D:611:GLN:C	1:D:613:GLN:N	2.76	0.42
1:A:299:ARG:HA	1:A:345:CYS:SG	2.60	0.42
1:A:503:LEU:HD12	1:A:503:LEU:HA	1.84	0.42
1:C:173:HIS:O	1:C:180:LEU:HB2	2.20	0.42
1:C:289:GLY:HA2	1:C:292:VAL:HG23	2.02	0.42
1:B:600:ILE:HG12	1:B:632:TRP:CZ2	2.54	0.42
1:B:611:GLN:HG3	2:B:846:HOH:O	2.20	0.42
1:B:683:ARG:O	1:B:688:LEU:HD22	2.19	0.42
1:D:61:ARG:NH2	1:D:477:ARG:HH12	2.18	0.42
1:C:68:SER:O	1:C:69:SER:OG	2.29	0.42
1:B:89:HIS:O	1:B:93:LEU:HD23	2.19	0.42
1:B:145:ILE:O	1:B:149:ARG:HG3	2.20	0.42
1:B:488:ALA:HA	1:B:497:VAL:O	2.19	0.42
1:D:388:LEU:HA	1:D:388:LEU:HD12	1.77	0.42
1:C:35:GLN:O	1:C:39:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:LEU:HA	1:C:388:LEU:HD12	1.81	0.42
1:C:725:GLU:O	1:C:725:GLU:HG3	2.18	0.42
1:B:43:LEU:H	1:B:43:LEU:HG	1.54	0.42
1:B:164:THR:HB	1:B:165:SER:H	1.52	0.42
1:D:459:MET:CE	1:D:501:ILE:HB	2.50	0.42
1:A:424:ALA:C	1:A:426:ALA:H	2.27	0.42
1:B:585:PRO:HA	1:B:588:ARG:HB2	2.01	0.42
1:A:230:HIS:CG	1:A:231:ASN:N	2.84	0.42
1:A:626:LEU:HD13	1:A:630:VAL:HG11	2.02	0.42
1:A:673:MET:HE1	1:A:690:ILE:CG2	2.50	0.42
1:B:189:ILE:HD13	1:B:189:ILE:HG21	1.83	0.42
1:B:525:ASP:HA	1:B:526:PRO:HD3	1.86	0.42
1:A:494:LEU:HD21	1:A:786:LEU:HD21	2.01	0.41
1:A:580:LEU:HD12	1:A:706:ALA:H	1.85	0.41
1:C:263:MET:HE2	1:C:263:MET:HB3	1.84	0.41
1:B:663:GLU:O	1:B:685:GLY:HA3	2.19	0.41
1:D:534:ILE:HG12	1:D:535:PRO:HD3	2.01	0.41
1:A:5:ASP:HB2	1:A:84:GLU:OE1	2.20	0.41
1:A:447:HIS:CG	1:A:790:LEU:HD21	2.55	0.41
1:C:321:LEU:HG	1:C:391:LEU:HD21	2.02	0.41
1:C:617:MET:HB3	1:C:632:TRP:CH2	2.55	0.41
1:B:9:THR:C	1:B:11:THR:N	2.77	0.41
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.84	0.41
1:B:563:PHE:CD2	1:B:649:ILE:HG13	2.55	0.41
1:B:753:LEU:HD22	1:B:757:TYR:HE2	1.85	0.41
1:D:590:LEU:HD23	1:D:590:LEU:HA	1.85	0.41
1:A:89:HIS:HE1	1:A:91:GLU:HB2	1.85	0.41
1:A:790:LEU:H	1:A:791:ALA:HB3	1.84	0.41
1:B:213:ILE:HD12	1:B:213:ILE:HA	1.88	0.41
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.89	0.41
1:D:89:HIS:O	1:D:93:LEU:HD23	2.20	0.41
1:D:301:LEU:HD12	1:D:301:LEU:HA	1.93	0.41
1:D:518:ASP:O	1:D:519:ILE:HD13	2.20	0.41
1:D:581:TYR:OH	1:D:592:ASN:HA	2.21	0.41
1:A:75:ALA:HB2	1:A:103:PHE:CZ	2.56	0.41
1:A:521:PHE:CZ	1:A:528:ARG:HB3	2.56	0.41
1:C:156:PHE:HE2	1:C:248:ALA:HB1	1.85	0.41
1:C:489:PHE:CZ	1:C:497:VAL:HG21	2.56	0.41
1:B:74:LEU:HD23	1:B:86:MET:HE2	2.02	0.41
1:B:718:LYS:O	1:B:722:ASN:HA	2.19	0.41
1:A:213:ILE:HD12	1:A:213:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:TRP:NE1	1:C:226:PRO:HB3	2.35	0.41
1:C:426:ALA:HA	1:C:482:GLN:OE1	2.19	0.41
1:C:720:LEU:HB2	1:C:723:PRO:HG3	2.03	0.41
1:D:10:CYS:O	1:D:10:CYS:SG	2.78	0.41
1:D:435:SER:HB3	1:D:448:PHE:CD2	2.56	0.41
1:D:561:LEU:HD22	1:D:594:VAL:CG2	2.51	0.41
1:A:145:ILE:O	1:A:149:ARG:HG3	2.21	0.41
1:C:21:LEU:HG	1:C:25:TYR:CE2	2.56	0.41
1:C:325:ARG:HD2	1:C:355:PHE:CZ	2.54	0.41
1:C:586:ARG:O	1:C:590:LEU:HD12	2.20	0.41
1:C:586:ARG:NH1	1:C:710:ASP:OD1	2.54	0.41
1:C:632:TRP:CD1	1:C:633:LEU:N	2.85	0.41
1:B:567:ARG:HA	1:B:567:ARG:HD2	1.82	0.41
1:D:181:MET:N	1:D:225:ALA:HB3	2.35	0.41
1:D:229:GLY:HA2	1:D:312:GLN:HA	2.02	0.41
1:D:603:GLN:HG3	1:D:614:ILE:CG2	2.50	0.41
1:C:167:LEU:HD23	1:C:167:LEU:HA	1.82	0.41
1:C:168:HIS:HB2	1:C:187:HIS:NE2	2.35	0.41
1:C:553:TYR:O	1:C:628:GLN:HA	2.20	0.41
1:D:48:ASP:HA	1:D:49:CYS:HA	1.55	0.41
1:D:531:HIS:HB3	1:D:532:SER:H	1.71	0.41
1:A:89:HIS:O	1:A:93:LEU:HD23	2.21	0.41
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.83	0.41
1:C:341:LYS:HB2	1:C:349:TRP:CZ3	2.55	0.41
1:B:44:GLN:H	1:B:46:GLU:N	2.19	0.41
1:D:278:GLN:NE2	1:D:342:VAL:HA	2.35	0.41
1:D:339:LEU:HD23	1:D:339:LEU:HA	1.71	0.41
1:D:559:LYS:HA	1:D:560:PRO:HD3	1.78	0.41
1:D:585:PRO:HG2	1:D:588:ARG:HG2	2.02	0.41
1:A:162:GLY:HA2	1:A:163:HIS:HA	1.75	0.41
1:A:215:LEU:CD2	1:A:232:ALA:HB2	2.50	0.41
1:C:328:PRO:CG	1:C:364:PRO:HA	2.49	0.41
1:C:459:MET:HE3	1:C:501:ILE:HB	2.02	0.41
1:C:534:ILE:HA	1:C:537:ILE:HD12	2.03	0.41
1:C:554:LEU:HA	1:C:628:GLN:HA	2.03	0.41
1:C:708:THR:O	1:C:712:ILE:HG13	2.21	0.41
1:B:99:THR:HG23	1:B:102:GLU:CD	2.45	0.41
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.84	0.41
1:B:550:ALA:HB1	1:B:631:ARG:HH12	1.85	0.41
1:B:582:ALA:HB1	1:B:624:HIS:ND1	2.36	0.41
1:B:624:HIS:HB2	1:B:626:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:LEU:HB3	1:B:635:MET:CE	2.50	0.41
1:D:263:MET:HE2	1:D:263:MET:HB2	1.77	0.41
1:A:45:THR:HB	1:A:48:ASP:O	2.20	0.41
1:C:593:LEU:HB3	1:C:630:VAL:HB	2.03	0.41
1:B:561:LEU:HD12	1:B:561:LEU:HA	1.82	0.41
1:A:28:ALA:HB1	1:A:30:ARG:O	2.20	0.40
1:C:13:GLN:O	1:C:14:ASN:HB2	2.21	0.40
1:B:686:GLY:O	1:B:690:ILE:HG13	2.21	0.40
1:D:76:LEU:HD22	1:D:86:MET:HE1	2.03	0.40
1:D:282:LEU:HB2	1:D:284:LEU:HG	2.03	0.40
1:D:657:VAL:HG22	1:D:680:PHE:HB2	2.03	0.40
1:A:281:VAL:HG11	1:A:291:VAL:HB	2.02	0.40
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.76	0.40
1:A:469:THR:HG1	1:A:472:GLU:HG3	1.83	0.40
1:A:742:THR:OG1	1:A:745:LEU:HB2	2.20	0.40
1:C:554:LEU:HG	1:C:631:ARG:HB2	2.04	0.40
1:C:563:PHE:CD1	1:C:564:THR:N	2.89	0.40
1:C:660:ALA:O	1:C:702:PRO:HG3	2.21	0.40
1:B:27:THR:O	1:B:27:THR:OG1	2.35	0.40
1:B:238:THR:O	1:B:241:MET:HB2	2.20	0.40
1:B:273:HIS:C	1:B:273:HIS:HD2	2.28	0.40
1:B:782:GLN:O	1:B:786:LEU:HG	2.21	0.40
1:D:275:TYR:H	1:D:287:THR:HG1	1.65	0.40
1:D:317:GLU:HA	1:D:318:PRO:HD2	1.90	0.40
1:A:34:LEU:HD22	1:A:433:LEU:HD13	2.02	0.40
1:A:69:SER:HB2	1:A:71:TRP:HB2	2.04	0.40
1:A:437:ILE:HD12	1:A:437:ILE:HA	1.88	0.40
1:A:715:PHE:HZ	1:A:726:TRP:CD1	2.38	0.40
1:C:225:ALA:HB1	1:C:226:PRO:HD2	2.03	0.40
1:C:265:SER:N	1:C:396:ASP:OD2	2.44	0.40
1:C:530:LEU:HD23	1:C:533:LEU:HD22	2.02	0.40
1:B:408:VAL:HG12	1:B:412:LEU:HD12	2.02	0.40
1:D:25:TYR:CZ	1:D:38:LEU:HD23	2.57	0.40
1:D:443:GLU:O	1:D:447:HIS:ND1	2.54	0.40
1:D:612:GLU:O	1:D:615:HIS:HB2	2.21	0.40
1:D:718:LYS:HB2	1:D:725:GLU:HB2	2.03	0.40
1:A:241:MET:O	1:A:245:ILE:HG13	2.21	0.40
1:A:604:HIS:CB	1:A:605:SER:HB3	2.51	0.40
1:A:661:LEU:HD12	1:A:661:LEU:HA	1.84	0.40
1:C:139:SER:O	1:C:142:GLN:HB2	2.20	0.40
1:B:587:LEU:HA	1:B:590:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LEU:HD22	1:B:757:TYR:CE2	2.56	0.40
1:A:521:PHE:HB2	1:A:522:PRO:CD	2.51	0.40
1:C:301:LEU:HD11	1:C:751:MET:HE3	2.04	0.40
1:B:230:HIS:CG	1:B:231:ASN:N	2.90	0.40
1:D:69:SER:OG	1:D:70:PRO:HD2	2.21	0.40
1:D:282:LEU:HD13	1:D:284:LEU:HD11	2.04	0.40
1:D:428:GLU:H	1:D:428:GLU:HG2	1.72	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	787/794 (99%)	707 (90%)	78 (10%)	2 (0%)	36	63
1	B	787/794 (99%)	699 (89%)	76 (10%)	12 (2%)	8	28
1	C	787/794 (99%)	713 (91%)	68 (9%)	6 (1%)	16	42
1	D	787/794 (99%)	692 (88%)	88 (11%)	7 (1%)	14	39
All	All	3148/3176 (99%)	2811 (89%)	310 (10%)	27 (1%)	14	39

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	ASN
1	B	160	GLU
1	B	189	ILE
1	C	11	THR
1	B	11	THR
1	B	69	SER
1	B	164	THR
1	D	158	ARG

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Mol	Chain	Res	Type
1	D	358	HIS
1	A	69	SER
1	C	12	GLN
1	D	69	SER
1	D	515	ALA
1	D	612	GLU
1	A	570	ARG
1	C	280	ASN
1	B	545	ALA
1	B	610	GLU
1	C	69	SER
1	B	281	VAL
1	B	611	GLN
1	D	156	PHE
1	B	600	ILE
1	D	609	GLU
1	B	557	PRO
1	C	601	ASP
1	B	659	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	673/687 (98%)	569 (84%)	104 (16%)	2	10
1	B	677/687 (98%)	576 (85%)	101 (15%)	3	11
1	C	680/687 (99%)	587 (86%)	93 (14%)	3	13
1	D	679/687 (99%)	569 (84%)	110 (16%)	2	9
All	All	2709/2748 (99%)	2301 (85%)	408 (15%)	3	11

All (408) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	THR

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Mol	Chain	Res	Type
1	A	11	THR
1	A	12	GLN
1	A	16	ASP
1	A	20	THR
1	A	29	ASN
1	A	48	ASP
1	A	55	LEU
1	A	68	SER
1	A	69	SER
1	A	74	LEU
1	A	84	GLU
1	A	86	MET
1	A	92	HIS
1	A	105	LYS
1	A	114	GLU
1	A	153	SER
1	A	163	HIS
1	A	165	SER
1	A	176	GLU
1	A	179	GLN
1	A	185	ASN
1	A	186	SER
1	A	194	ASN
1	A	200	LEU
1	A	201	GLU
1	A	202	MET
1	A	215	LEU
1	A	218	LYS
1	A	241	MET
1	A	243	MET
1	A	256	GLU
1	A	263	MET
1	A	266	ARG
1	A	270	LEU
1	A	278	GLN
1	A	281	VAL
1	A	297	GLN
1	A	301	LEU
1	A	305	MET
1	A	308	ARG
1	A	309	LEU
1	A	311	LEU

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Mol	Chain	Res	Type
1	A	314	VAL
1	A	332	ASP
1	A	334	THR
1	A	339	LEU
1	A	341	LYS
1	A	362	ILE
1	A	369	ARG
1	A	371	GLU
1	A	388	LEU
1	A	391	LEU
1	A	404	ASP
1	A	407	LEU
1	A	413	SER
1	A	429	LYS
1	A	430	THR
1	A	441	GLU
1	A	457	LEU
1	A	464	PHE
1	A	471	GLN
1	A	501	ILE
1	A	503	LEU
1	A	525	ASP
1	A	527	ASN
1	A	528	ARG
1	A	530	LEU
1	A	533	LEU
1	A	547	ASN
1	A	548	LEU
1	A	553	TYR
1	A	554	LEU
1	A	556	ASP
1	A	561	LEU
1	A	570	ARG
1	A	579	GLU
1	A	580	LEU
1	A	589	SER
1	A	594	VAL
1	A	595	ILE
1	A	614	ILE
1	A	620	LEU
1	A	628	GLN
1	A	629	GLN

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Mol	Chain	Res	Type
1	A	636	ARG
1	A	637	LEU
1	A	638	ASP
1	A	639	LYS
1	A	658	GLN
1	A	661	LEU
1	A	662	PHE
1	A	667	LEU
1	A	682	THR
1	A	687	PRO
1	A	691	ILE
1	A	696	SER
1	A	745	LEU
1	A	766	LEU
1	A	772	ASP
1	A	773	ARG
1	A	784	ARG
1	A	790	LEU
1	C	4	ILE
1	C	5	ASP
1	C	9	THR
1	C	29	ASN
1	C	31	THR
1	C	32	LEU
1	C	34	LEU
1	C	44	GLN
1	C	53	ASP
1	C	55	LEU
1	C	64	GLU
1	C	74	LEU
1	C	86	MET
1	C	91	GLU
1	C	93	LEU
1	C	94	ILE
1	C	111	VAL
1	C	116	THR
1	C	119	VAL
1	C	138	ARG
1	C	157	SER
1	C	165	SER
1	C	175	ILE
1	C	179	GLN

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Mol	Chain	Res	Type
1	C	187	HIS
1	C	197	ARG
1	C	200	LEU
1	C	207	ASP
1	C	209	THR
1	C	220	ASN
1	C	255	GLU
1	C	267	LEU
1	C	270	LEU
1	C	273	HIS
1	C	280	ASN
1	C	301	LEU
1	C	309	LEU
1	C	311	LEU
1	C	312	GLN
1	C	314	VAL
1	C	316	VAL
1	C	319	LYS
1	C	356	ARG
1	C	363	ILE
1	C	368	SER
1	C	378	ILE
1	C	386	GLU
1	C	388	LEU
1	C	404	ASP
1	C	407	LEU
1	C	430	THR
1	C	435	SER
1	C	440	GLN
1	C	457	LEU
1	C	471	GLN
1	C	478	GLU
1	C	490	SER
1	C	497	VAL
1	C	503	LEU
1	C	525	ASP
1	C	530	LEU
1	C	534	ILE
1	C	536	GLU
1	C	541	ILE
1	C	551	ARG
1	C	553	TYR

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Mol	Chain	Res	Type
1	C	558	ASP
1	C	559	LYS
1	C	564	THR
1	C	568	LEU
1	C	571	ILE
1	C	575	THR
1	C	590	LEU
1	C	601	ASP
1	C	604	HIS
1	C	606	SER
1	C	608	HIS
1	C	612	GLU
1	C	615	HIS
1	C	617	MET
1	C	627	ASP
1	C	628	GLN
1	C	630	VAL
1	C	640	ASN
1	C	667	LEU
1	C	710	ASP
1	C	711	LEU
1	C	725	GLU
1	C	740	ARG
1	C	745	LEU
1	C	763	VAL
1	C	766	LEU
1	C	784	ARG
1	B	9	THR
1	B	10	CYS
1	B	15	ARG
1	B	23	ARG
1	B	26	PHE
1	B	29	ASN
1	B	30	ARG
1	B	43	LEU
1	B	45	THR
1	B	47	GLN
1	B	48	ASP
1	B	49	CYS
1	B	55	LEU
1	B	68	SER
1	B	74	LEU

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Mol	Chain	Res	Type
1	B	92	HIS
1	B	93	LEU
1	B	99	THR
1	B	100	ILE
1	B	110	VAL
1	B	114	GLU
1	B	116	THR
1	B	142	GLN
1	B	153	SER
1	B	154	GLU
1	B	157	SER
1	B	158	ARG
1	B	200	LEU
1	B	209	THR
1	B	213	ILE
1	B	222	LEU
1	B	245	ILE
1	B	270	LEU
1	B	273	HIS
1	B	291	VAL
1	B	295	LEU
1	B	305	MET
1	B	308	ARG
1	B	309	LEU
1	B	314	VAL
1	B	316	VAL
1	B	317	GLU
1	B	324	THR
1	B	334	THR
1	B	339	LEU
1	B	361	GLU
1	B	369	ARG
1	B	371	GLU
1	B	388	LEU
1	B	404	ASP
1	B	407	LEU
1	B	413	SER
1	B	430	THR
1	B	431	LYS
1	B	433	LEU
1	B	435	SER
1	B	437	ILE

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Mol	Chain	Res	Type
1	B	444	ASP
1	B	457	LEU
1	B	469	THR
1	B	503	LEU
1	B	507	LYS
1	B	525	ASP
1	B	530	LEU
1	B	532	SER
1	B	533	LEU
1	B	534	ILE
1	B	536	GLU
1	B	546	THR
1	B	547	ASN
1	B	548	LEU
1	B	556	ASP
1	B	558	ASP
1	B	561	LEU
1	B	569	ASP
1	B	570	ARG
1	B	571	ILE
1	B	595	ILE
1	B	607	ASP
1	B	610	GLU
1	B	612	GLU
1	B	617	MET
1	B	619	GLN
1	B	620	LEU
1	B	622	ASP
1	B	630	VAL
1	B	640	ASN
1	B	652	LYS
1	B	661	LEU
1	B	667	LEU
1	B	677	LEU
1	B	688	LEU
1	B	693	ASN
1	B	708	THR
1	B	719	ASN
1	B	740	ARG
1	B	745	LEU
1	B	748	GLU
1	B	754	SER

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Mol	Chain	Res	Type
1	B	773	ARG
1	B	784	ARG
1	D	4	ILE
1	D	12	GLN
1	D	31	THR
1	D	32	LEU
1	D	36	SER
1	D	40	GLU
1	D	42	LEU
1	D	44	GLN
1	D	45	THR
1	D	46	GLU
1	D	54	MET
1	D	60	PHE
1	D	68	SER
1	D	69	SER
1	D	80	ILE
1	D	88	ILE
1	D	92	HIS
1	D	99	THR
1	D	114	GLU
1	D	116	THR
1	D	119	VAL
1	D	135	LYS
1	D	137	SER
1	D	139	SER
1	D	145	ILE
1	D	150	LYS
1	D	152	SER
1	D	153	SER
1	D	159	ILE
1	D	163	HIS
1	D	164	THR
1	D	180	LEU
1	D	197	ARG
1	D	200	LEU
1	D	202	MET
1	D	203	LEU
1	D	206	LEU
1	D	209	THR
1	D	218	LYS
1	D	237	GLU

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Mol	Chain	Res	Type
1	D	241	MET
1	D	255	GLU
1	D	260	CYS
1	D	263	MET
1	D	273	HIS
1	D	280	ASN
1	D	282	LEU
1	D	290	GLN
1	D	295	LEU
1	D	297	GLN
1	D	308	ARG
1	D	309	LEU
1	D	311	LEU
1	D	316	VAL
1	D	320	ILE
1	D	334	THR
1	D	343	SER
1	D	362	ILE
1	D	372	ILE
1	D	385	ARG
1	D	388	LEU
1	D	430	THR
1	D	433	LEU
1	D	456	LEU
1	D	457	LEU
1	D	471	GLN
1	D	476	THR
1	D	478	GLU
1	D	491	MET
1	D	501	ILE
1	D	525	ASP
1	D	530	LEU
1	D	534	ILE
1	D	538	GLU
1	D	540	LEU
1	D	555	GLN
1	D	556	ASP
1	D	561	LEU
1	D	568	LEU
1	D	574	ILE
1	D	575	THR
1	D	577	LEU

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Mol	Chain	Res	Type
1	D	580	LEU
1	D	587	LEU
1	D	600	ILE
1	D	601	ASP
1	D	605	SER
1	D	617	MET
1	D	620	LEU
1	D	621	MET
1	D	625	GLU
1	D	640	ASN
1	D	647	ARG
1	D	648	TYR
1	D	652	LYS
1	D	653	ARG
1	D	658	GLN
1	D	667	LEU
1	D	682	THR
1	D	691	ILE
1	D	696	SER
1	D	712	ILE
1	D	721	GLU
1	D	728	ARG
1	D	730	SER
1	D	734	LEU
1	D	742	THR
1	D	763	VAL
1	D	770	GLU
1	D	784	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	168	HIS
1	A	185	ASN
1	A	273	HIS
1	A	394	HIS
1	A	420	GLN
1	A	531	HIS
1	A	780	HIS
1	A	782	GLN
1	C	173	HIS

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Mol	Chain	Res	Type
1	C	194	ASN
1	C	220	ASN
1	C	290	GLN
1	C	310	GLN
1	C	401	ASN
1	C	442	ASN
1	C	487	GLN
1	C	603	GLN
1	C	615	HIS
1	C	640	ASN
1	C	719	ASN
1	B	92	HIS
1	B	184	ASN
1	B	190	HIS
1	B	233	ASN
1	B	358	HIS
1	B	359	ASN
1	B	406	ASN
1	B	619	GLN
1	B	629	GLN
1	B	719	ASN
1	D	12	GLN
1	D	44	GLN
1	D	63	GLN
1	D	90	GLN
1	D	92	HIS
1	D	185	ASN
1	D	187	HIS
1	D	198	GLN
1	D	233	ASN
1	D	401	ASN
1	D	471	GLN
1	D	603	GLN
1	D	618	HIS
1	D	776	ASN
1	D	782	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	A	789/794 (99%)	-0.52	14 (1%)	67 45	8, 37, 104, 170	0
1	B	789/794 (99%)	-0.53	15 (1%)	66 43	9, 38, 103, 152	0
1	C	789/794 (99%)	-0.41	15 (1%)	66 43	10, 46, 111, 167	0
1	D	789/794 (99%)	-0.08	42 (5%)	32 16	11, 60, 140, 180	0
All	All	3156/3176 (99%)	-0.39	86 (2%)	56 33	8, 44, 116, 180	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	LEU	7.3
1	D	562	ILE	6.5
1	D	549	PRO	5.3
1	A	602	PRO	4.6
1	D	282	LEU	4.5
1	D	599	LYS	4.4
1	D	597	GLY	4.2
1	D	792	HIS	4.1
1	C	4	ILE	4.1
1	D	533	LEU	3.9
1	A	601	ASP	3.9
1	B	282	LEU	3.8
1	D	590	LEU	3.7
1	D	537	ILE	3.7
1	A	281	VAL	3.6
1	A	608	HIS	3.6
1	B	28	ALA	3.4
1	D	720	LEU	3.4
1	D	564	THR	3.4
1	C	281	VAL	3.2
1	D	550	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	719	ASN	3.2
1	D	630	VAL	3.2
1	C	282	LEU	3.1
1	B	548	LEU	3.1
1	D	715	PHE	3.1
1	D	541	ILE	3.1
1	D	563	PHE	3.0
1	A	610	GLU	3.0
1	D	534	ILE	3.0
1	D	600	ILE	3.0
1	C	545	ALA	3.0
1	C	332	ASP	3.0
1	D	653	ARG	2.9
1	A	159	ILE	2.9
1	B	720	LEU	2.9
1	D	632	TRP	2.9
1	D	535	PRO	2.9
1	B	31	THR	2.8
1	B	658	GLN	2.8
1	D	580	LEU	2.7
1	D	530	LEU	2.7
1	D	593	LEU	2.7
1	D	566	ALA	2.7
1	D	595	ILE	2.7
1	A	4	ILE	2.6
1	D	655	ILE	2.6
1	D	645	LEU	2.6
1	D	626	LEU	2.6
1	C	187	HIS	2.6
1	D	45	THR	2.6
1	D	557	PRO	2.5
1	B	587	LEU	2.5
1	A	164	THR	2.5
1	C	611	GLN	2.5
1	A	607	ASP	2.5
1	D	542	PHE	2.4
1	D	43	LEU	2.4
1	D	641	LEU	2.4
1	D	560	PRO	2.4
1	C	531	HIS	2.4
1	B	187	HIS	2.4
1	C	610	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	550	ALA	2.4
1	A	706	ALA	2.3
1	D	4	ILE	2.3
1	C	620	LEU	2.3
1	B	281	VAL	2.3
1	D	649	ILE	2.3
1	A	186	SER	2.3
1	D	602	PRO	2.3
1	B	791	ALA	2.3
1	A	187	HIS	2.2
1	D	545	ALA	2.2
1	B	280	ASN	2.2
1	B	549	PRO	2.2
1	D	164	THR	2.1
1	D	598	GLY	2.1
1	C	549	PRO	2.1
1	B	584	SER	2.1
1	C	558	ASP	2.1
1	D	42	LEU	2.1
1	A	611	GLN	2.1
1	B	49	CYS	2.1
1	B	186	SER	2.0
1	C	330	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.