Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 06:41 AM EDT

PDB ID	:	5K8D
Title	:	Crystal structure of rFVIIIFc
Authors	:	Leksa, N.; Quan, C.
Deposited on	:	2016-05-29
Resolution	:	4.19 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 (i) 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 (i)) were used in the production of this report:

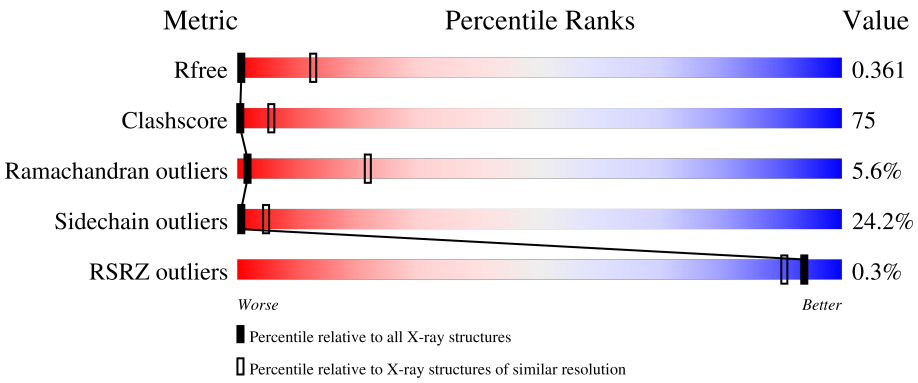
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 <=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	740	21% 45% 16% • 17%
2	B	865	20% 36% 15% • 28%
3	C	4	25% 75%
4	D	2	100%
5	E	7	14% 43% 43%

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
3	BMA	C	3	-	-	X	-
4	NAG	D	1	-	-	-	X
4	NAG	D	2	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10138 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 Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	611	4937	3190	824	898	25	0	0	0

- Molecule 2 is a protein called Coagulation factor VIII,Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	5035	3234	862	908	31	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2332	TYR	-	linker	UNP P00451

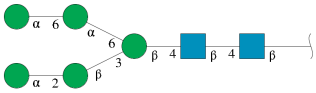
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	50	28	2	20	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	7	83	46	2	35	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	3	3	3	0	0

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

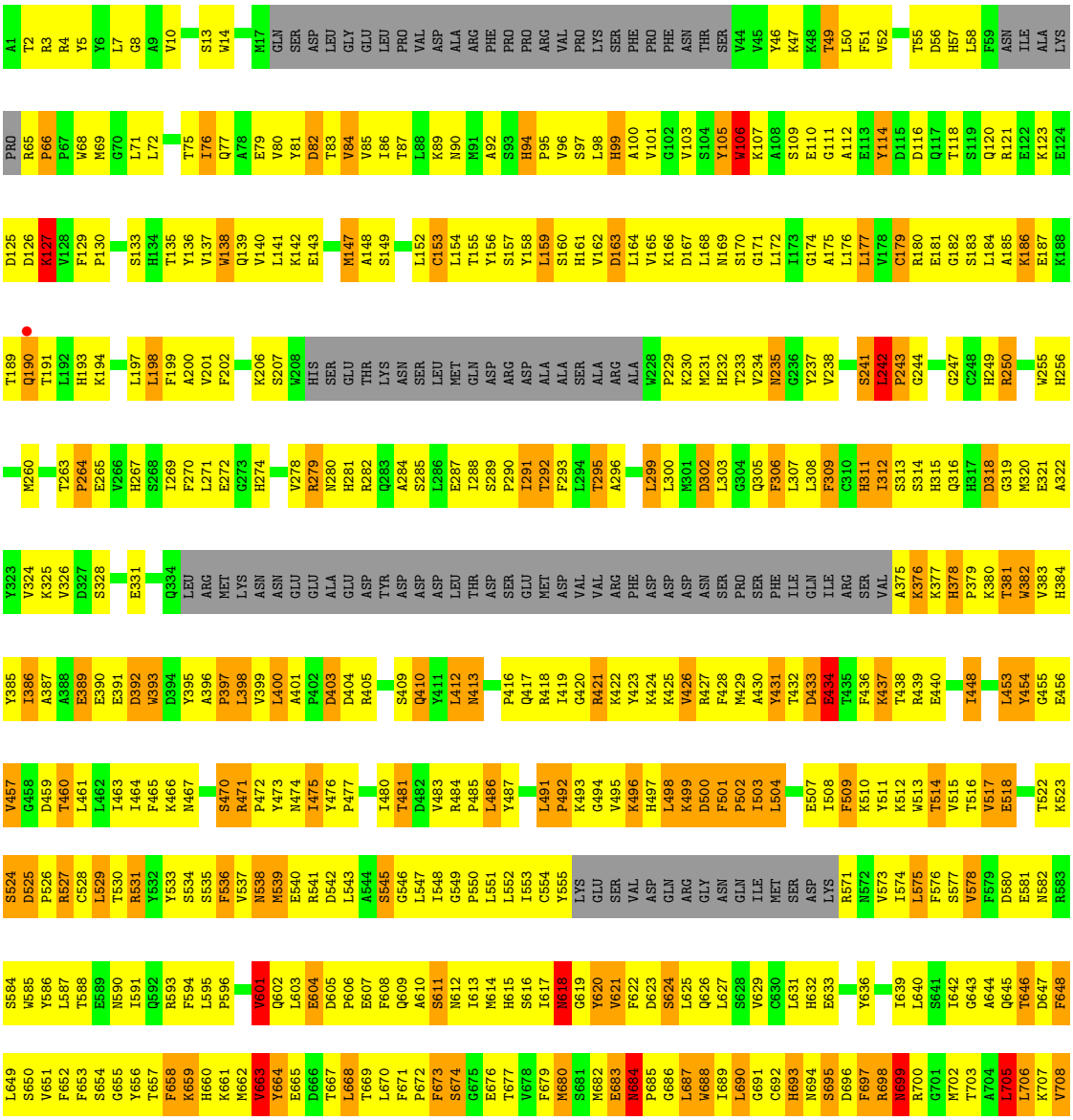
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
7	A	1	1	1	0	0
7	B	1	1	1	0	0

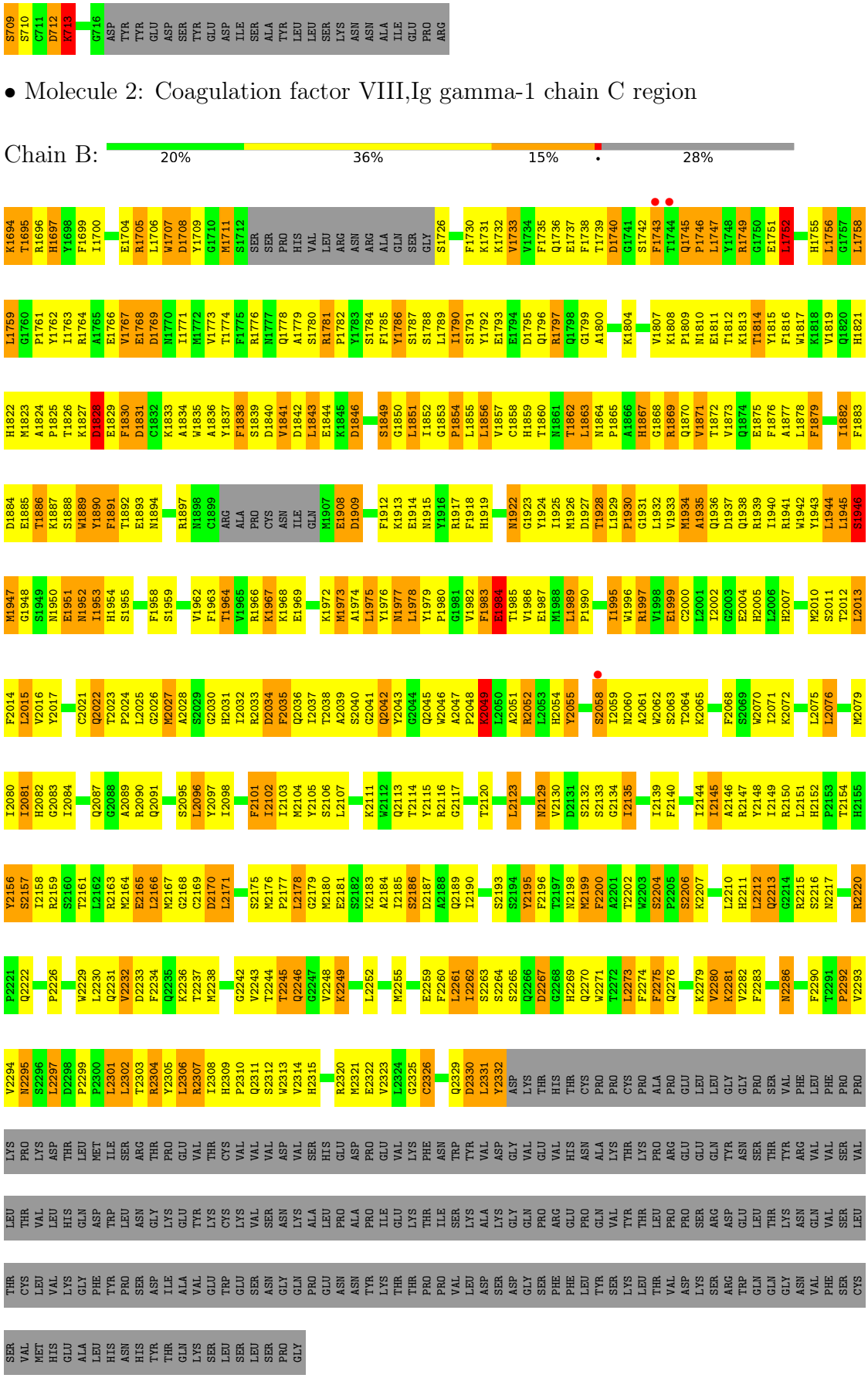
3 Residue-property plots (i)

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: Coagulation factor VIII

Chain A: 21% 45% 16% • 17%

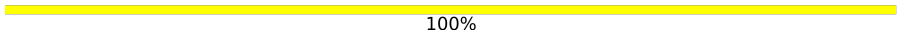



S709 S710 C711 D712 K713 G716 ASP TYR TYR GLU ASP SER TYR GLU ASP ILE SER ALA TYR LEU LEU SER LYS ASN ASN ALA ILE GLU PRO ARG
• Molecule 2: Coagulation factor VIII,Ig gamma-1 chain C region
Chain B:
20%
36%
15%
28%

• Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

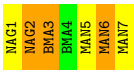
Chain C:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

• Molecule 5: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	136.29Å 136.29Å 365.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.60 – 4.19 37.60 – 4.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.60-4.19) 99.0 (37.60-4.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.298 , 0.362 0.298 , 0.361	Depositor DCC
R_{free} test set	1309 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	126.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 131.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	10138	wwPDB-VP
Average B, all atoms (Å^2)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, BMA, CA, CU

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	0.86	15/5077 (0.3%)	0.90	4/6890 (0.1%)
2	B	0.80	21/5178 (0.4%)	0.86	1/7011 (0.0%)
All	All	0.83	36/10255 (0.4%)	0.88	5/13901 (0.0%)

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	2
2	B	0	2
All	All	0	4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	GLU	CD-OE1	14.90	1.42	1.25
1	A	389	GLU	CD-OE2	14.10	1.41	1.25
1	A	697	PHE	CG-CD2	13.56	1.59	1.38
1	A	697	PHE	CG-CD1	11.83	1.56	1.38
1	A	697	PHE	CE1-CZ	10.48	1.57	1.37
2	B	1838	PHE	CG-CD1	9.46	1.52	1.38
1	A	434	GLU	CD-OE2	9.38	1.35	1.25
2	B	1983	PHE	CG-CD1	9.21	1.52	1.38
1	A	434	GLU	CG-CD	9.06	1.65	1.51
1	A	697	PHE	CE2-CZ	8.83	1.54	1.37
2	B	1983	PHE	CG-CD2	8.79	1.51	1.38
2	B	1897	ARG	NE-CZ	8.15	1.43	1.33
2	B	1742	SER	CB-OG	8.09	1.52	1.42
2	B	2055	TYR	CE1-CZ	7.83	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	712	ASP	CG-OD2	7.58	1.42	1.25
2	B	1838	PHE	CG-CD2	7.37	1.49	1.38
2	B	1743	PHE	CG-CD1	7.34	1.49	1.38
2	B	1983	PHE	CE2-CZ	7.33	1.51	1.37
1	A	712	ASP	CG-OD1	7.30	1.42	1.25
2	B	1983	PHE	CE1-CZ	7.30	1.51	1.37
2	B	1745	GLN	CG-CD	7.25	1.67	1.51
1	A	389	GLU	CG-CD	7.24	1.62	1.51
1	A	389	GLU	CD-OE1	6.81	1.33	1.25
2	B	1838	PHE	CE2-CZ	6.40	1.49	1.37
1	A	190	GLN	CG-CD	6.35	1.65	1.51
1	A	618	ASN	C-O	6.15	1.35	1.23
2	B	1838	PHE	CE1-CZ	6.05	1.48	1.37
2	B	2055	TYR	CG-CD2	6.04	1.47	1.39
2	B	1946	SER	CB-OG	5.94	1.50	1.42
2	B	1743	PHE	CG-CD2	5.89	1.47	1.38
2	B	2058	SER	CB-OG	5.71	1.49	1.42
2	B	1897	ARG	CZ-NH2	5.51	1.40	1.33
2	B	2330	ASP	CG-OD1	5.27	1.37	1.25
2	B	2267	ASP	CG-OD2	5.09	1.37	1.25
2	B	1983	PHE	CD1-CE1	5.09	1.49	1.39
1	A	712	ASP	CB-CG	5.04	1.62	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	LEU	C-N-CD	-6.36	106.62	120.60
1	A	179	CYS	CA-CB-SG	-5.99	103.21	114.00
2	B	2330	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	A	186	LYS	CD-CE-NZ	5.28	123.84	111.70
1	A	250	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	ALA	Peptide
1	A	693	HIS	Peptide
2	B	1790	ILE	Peptide
2	B	1828	ASP	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	4937	0	4820	803	1
2	B	5035	0	4902	791	0
3	C	50	0	43	8	0
4	D	28	0	25	0	0
5	E	83	0	70	4	0
6	A	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	10138	0	9860	1508	1

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 75.

All (1508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2046:TRP:CZ3	2:B:2059:ILE:HA	1.37	1.59
1:A:287:GLU:HB3	1:A:673:PHE:CE2	1.51	1.42
2:B:1934:MET:CE	2:B:1940:ILE:HD13	1.46	1.41
2:B:1738:PHE:CD2	2:B:1747:LEU:HD12	1.57	1.36
1:A:65:ARG:CG	1:A:66:PRO:HD3	1.57	1.35
2:B:1738:PHE:CB	2:B:1746:PRO:O	1.75	1.34
2:B:1738:PHE:HB2	2:B:1746:PRO:O	1.19	1.33
2:B:1830:PHE:CD1	2:B:1966:ARG:NH1	2.03	1.26
1:A:114:TYR:CE2	2:B:1997:ARG:HB2	1.69	1.26
2:B:1758:LEU:HD11	2:B:1923:GLY:CA	1.63	1.25
2:B:1786:TYR:HA	2:B:1790:ILE:CD1	1.65	1.25
2:B:1944:LEU:O	2:B:1978:LEU:HD11	1.29	1.25
1:A:395:TYR:HB3	1:A:621:VAL:CG2	1.65	1.25
2:B:2180:MET:HB2	2:B:2322:GLU:OE2	1.32	1.25
2:B:1828:ASP:OD2	2:B:1968:LYS:HA	1.31	1.23
1:A:625:LEU:CD1	1:A:706:LEU:HD11	1.68	1.23
1:A:5:TYR:CE2	1:A:76:ILE:HB	1.72	1.22
2:B:2264:SER:OG	2:B:2301:LEU:HD21	1.35	1.21
2:B:1945:LEU:HG	2:B:1983:PHE:CB	1.68	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD21	1:A:533:TYR:CE2	1.75	1.20
2:B:2046:TRP:CZ3	2:B:2059:ILE:CA	2.24	1.18
1:A:417:GLN:OE1	1:A:601:VAL:HG22	1.39	1.18
1:A:657:THR:HG21	2:B:1788:SER:HA	1.25	1.17
2:B:1830:PHE:HD1	2:B:1966:ARG:NH1	1.40	1.17
2:B:1813:LYS:HD2	2:B:1814:THR:H	1.04	1.17
2:B:1945:LEU:CG	2:B:1983:PHE:HB2	1.75	1.16
2:B:2046:TRP:CH2	2:B:2059:ILE:HA	1.81	1.15
2:B:2032:ILE:HG23	2:B:2036:GLN:OE1	1.43	1.15
2:B:2046:TRP:HH2	2:B:2058:SER:O	1.27	1.15
1:A:114:TYR:CD2	2:B:1997:ARG:HD3	1.82	1.14
1:A:395:TYR:CB	1:A:621:VAL:CG2	2.26	1.14
2:B:1947:MET:HE2	2:B:1948:GLY:H	1.07	1.13
2:B:2329:GLN:HG3	2:B:2332:TYR:O	1.44	1.13
2:B:2052:ARG:HD3	2:B:2165:GLU:HB2	1.25	1.12
2:B:2087:GLN:HB3	2:B:2163:ARG:HB2	1.13	1.12
1:A:651:VAL:H	1:A:693:HIS:HB2	1.09	1.12
2:B:1946:SER:CB	2:B:1978:LEU:HD12	1.80	1.12
1:A:621:VAL:HG12	1:A:622:PHE:H	1.07	1.11
1:A:625:LEU:HD13	1:A:706:LEU:CG	1.79	1.11
1:A:105:TYR:HB3	1:A:109:SER:HB3	1.29	1.11
1:A:663:VAL:HG22	2:B:1968:LYS:HD2	1.21	1.10
2:B:1886:THR:CG2	2:B:1913:LYS:NZ	2.16	1.09
2:B:1947:MET:CE	2:B:1948:GLY:H	1.65	1.09
2:B:2083:GLY:HA2	2:B:2140:PHE:CD2	1.87	1.09
2:B:1758:LEU:HD11	2:B:1923:GLY:HA3	1.09	1.09
2:B:1886:THR:HG21	2:B:1913:LYS:NZ	1.67	1.09
2:B:1934:MET:HE2	2:B:1940:ILE:CD1	1.82	1.09
2:B:1786:TYR:HA	2:B:1790:ILE:HD11	1.18	1.08
2:B:2330:ASP:HB3	2:B:2331:LEU:HD23	1.32	1.08
1:A:700:ARG:HH22	2:B:1844:GLU:CB	1.67	1.07
2:B:1891:PHE:HD1	2:B:1892:THR:N	1.51	1.07
2:B:1945:LEU:HA	2:B:1983:PHE:HA	1.27	1.07
2:B:2087:GLN:CB	2:B:2163:ARG:HB2	1.84	1.07
2:B:1743:PHE:CE1	2:B:1778:GLN:NE2	2.21	1.07
2:B:1886:THR:HG21	2:B:1913:LYS:HZ3	0.92	1.07
1:A:75:THR:HG22	1:A:175:ALA:HB3	1.37	1.07
1:A:287:GLU:CB	1:A:673:PHE:CE2	2.37	1.07
2:B:1813:LYS:HD2	2:B:1814:THR:N	1.68	1.06
2:B:2169:CYS:O	2:B:2170:ASP:HB3	1.34	1.06
2:B:2187:ASP:HB2	2:B:2206:SER:HB3	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:CG	1:A:66:PRO:CD	2.33	1.06
1:A:5:TYR:HE2	1:A:76:ILE:HB	1.07	1.06
1:A:148:ALA:HA	1:A:180:ARG:NH2	1.69	1.06
2:B:1934:MET:CE	2:B:1940:ILE:CD1	2.34	1.06
1:A:100:ALA:HB2	1:A:138:TRP:CZ3	1.90	1.05
1:A:395:TYR:HB3	1:A:621:VAL:HG23	1.07	1.05
2:B:1828:ASP:OD2	2:B:1968:LYS:CA	2.03	1.05
2:B:1886:THR:CG2	2:B:1913:LYS:HZ3	1.67	1.05
2:B:1934:MET:HE2	2:B:1940:ILE:HD13	1.07	1.05
1:A:471:ARG:HG2	1:A:585:TRP:CE3	1.91	1.05
2:B:2052:ARG:CD	2:B:2165:GLU:HB2	1.87	1.05
1:A:65:ARG:HG2	1:A:66:PRO:HD3	1.12	1.05
2:B:1707:TRP:HE1	2:B:1758:LEU:HD21	1.18	1.05
2:B:1838:PHE:HZ	2:B:1947:MET:HG3	1.15	1.04
1:A:141:LEU:HD23	1:A:143:GLU:H	1.22	1.03
2:B:1963:PHE:CD1	2:B:1986:VAL:HG11	1.94	1.03
2:B:2096:LEU:HB3	2:B:2161:THR:HG21	1.08	1.03
2:B:2273:LEU:HD21	2:B:2280:VAL:CG2	1.88	1.03
1:A:491:LEU:O	1:A:493:LYS:N	1.92	1.02
1:A:625:LEU:CD1	1:A:706:LEU:CD1	2.36	1.02
2:B:1790:ILE:HA	2:B:1817:TRP:CE3	1.95	1.02
2:B:1909:ASP:O	2:B:1913:LYS:HB2	1.58	1.02
2:B:2273:LEU:HD21	2:B:2280:VAL:HG21	1.36	1.02
1:A:531:ARG:HB2	1:A:551:LEU:O	1.58	1.01
1:A:700:ARG:HH22	2:B:1844:GLU:HB2	1.20	1.01
1:A:615:HIS:HB2	1:A:703:THR:HB	1.40	1.01
1:A:662:MET:HG3	1:A:680:MET:HE1	1.39	1.01
2:B:1946:SER:HB3	2:B:1978:LEU:HD12	1.36	1.01
2:B:1983:PHE:CD1	2:B:1984:GLU:N	2.29	1.01
2:B:2038:THR:HG21	2:B:2072:LYS:HE2	1.42	1.01
1:A:432:THR:OG1	1:A:440:GLU:HB3	1.61	1.01
2:B:1758:LEU:HD11	2:B:1923:GLY:N	1.75	1.01
1:A:622:PHE:O	1:A:705:LEU:HB2	1.60	1.00
2:B:1707:TRP:NE1	2:B:1758:LEU:CD2	2.24	0.99
1:A:395:TYR:HB2	1:A:621:VAL:HG21	1.45	0.99
2:B:1829:GLU:H	2:B:1966:ARG:HD2	1.26	0.99
2:B:2083:GLY:HA2	2:B:2140:PHE:HD2	1.22	0.98
1:A:287:GLU:HB3	1:A:673:PHE:CD2	1.97	0.98
1:A:625:LEU:HD13	1:A:706:LEU:CD1	1.91	0.98
2:B:1758:LEU:CD1	2:B:1923:GLY:HA3	1.92	0.98
1:A:663:VAL:CG2	2:B:1968:LYS:HD2	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2046:TRP:CH2	2:B:2058:SER:O	2.17	0.98
2:B:2306:LEU:HD23	2:B:2307:ARG:H	1.25	0.98
1:A:389:GLU:OE1	1:A:431:TYR:CE2	2.16	0.98
2:B:2052:ARG:H	2:B:2163:ARG:HB3	1.25	0.98
2:B:2169:CYS:O	2:B:2170:ASP:CB	2.09	0.97
2:B:2329:GLN:O	2:B:2332:TYR:O	1.81	0.97
1:A:622:PHE:CE1	1:A:702:MET:O	2.16	0.97
1:A:617:ILE:O	1:A:618:ASN:HB2	1.60	0.97
2:B:1946:SER:HB3	2:B:1978:LEU:CD1	1.94	0.97
2:B:1964:THR:O	2:B:1986:VAL:HG13	1.64	0.97
1:A:180:ARG:O	1:A:183:SER:HB3	1.65	0.96
1:A:625:LEU:HD13	1:A:706:LEU:HG	1.43	0.96
2:B:1944:LEU:O	2:B:1978:LEU:CD1	2.12	0.96
2:B:1738:PHE:HD2	2:B:1747:LEU:HD12	0.91	0.96
2:B:1934:MET:HB3	2:B:2016:VAL:HB	1.45	0.96
2:B:1934:MET:HE3	2:B:1940:ILE:HD13	1.42	0.96
1:A:287:GLU:HB3	1:A:673:PHE:HE2	1.15	0.96
2:B:1829:GLU:H	2:B:1966:ARG:CD	1.79	0.96
1:A:433:ASP:O	1:A:434:GLU:HG3	1.65	0.95
2:B:2051:ALA:HB1	2:B:2164:MET:H	1.31	0.95
1:A:398:LEU:HD23	1:A:399:VAL:HG12	1.43	0.95
1:A:656:TYR:CZ	2:B:1791:SER:HB2	2.01	0.95
1:A:642:ILE:HG22	1:A:643:GLY:H	1.29	0.95
3:C:3:BMA:H61	3:C:4:MAN:H3	1.45	0.95
1:A:114:TYR:HE2	2:B:1997:ARG:HB2	1.01	0.95
1:A:501:PHE:O	1:A:503:ILE:HG12	1.64	0.95
1:A:663:VAL:HG22	2:B:1968:LYS:CD	1.95	0.95
2:B:2273:LEU:CD2	2:B:2280:VAL:CG2	2.45	0.94
1:A:312:ILE:HD12	1:A:315:HIS:CE1	2.03	0.94
2:B:1829:GLU:N	2:B:1966:ARG:HD2	1.82	0.94
2:B:2034:ASP:HB3	2:B:2049:LYS:HD2	1.49	0.94
2:B:2087:GLN:HB3	2:B:2163:ARG:CB	1.97	0.94
2:B:2264:SER:CB	2:B:2301:LEU:CD2	2.46	0.94
1:A:395:TYR:CB	1:A:621:VAL:HG21	1.94	0.94
1:A:187:GLU:HA	1:A:190:GLN:HB3	1.47	0.94
2:B:2046:TRP:HZ3	2:B:2060:ASN:N	1.65	0.94
2:B:1738:PHE:HB3	2:B:1746:PRO:O	1.67	0.94
1:A:10:VAL:HG23	1:A:52:VAL:HG21	1.50	0.93
2:B:1838:PHE:CZ	2:B:1947:MET:HG3	2.02	0.93
1:A:109:SER:HB2	1:A:137:VAL:O	1.68	0.93
1:A:617:ILE:HD13	1:A:706:LEU:HD13	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:PHE:HD1	1:A:306:PHE:N	1.65	0.93
2:B:2096:LEU:HB3	2:B:2161:THR:CG2	1.99	0.93
1:A:700:ARG:NH2	2:B:1844:GLU:HB2	1.83	0.93
2:B:2046:TRP:HZ3	2:B:2059:ILE:CA	1.70	0.93
2:B:1829:GLU:HB2	2:B:1966:ARG:HD2	1.51	0.93
2:B:2052:ARG:HD3	2:B:2165:GLU:CB	1.98	0.92
1:A:114:TYR:HD2	2:B:1997:ARG:HD3	1.24	0.92
1:A:114:TYR:HE2	2:B:1997:ARG:CB	1.80	0.92
2:B:1743:PHE:HE1	2:B:1778:GLN:CD	1.72	0.92
1:A:157:SER:HB2	1:A:174:GLY:O	1.67	0.92
1:A:498:LEU:HD12	1:A:498:LEU:H	1.32	0.92
1:A:656:TYR:CB	1:A:686:GLY:HA2	1.99	0.92
1:A:615:HIS:HB2	1:A:703:THR:CB	2.00	0.91
2:B:1707:TRP:NE1	2:B:1758:LEU:HD21	1.83	0.91
2:B:1738:PHE:CD2	2:B:1747:LEU:CD1	2.51	0.91
2:B:2039:ALA:HB2	2:B:2048:PRO:HG2	1.49	0.91
1:A:688:TRP:HE1	2:B:1800:ALA:N	1.68	0.91
2:B:1789:LEU:HD23	2:B:1823:MET:HB3	1.53	0.91
2:B:1946:SER:HB3	2:B:1978:LEU:HB3	1.50	0.91
1:A:287:GLU:CB	1:A:673:PHE:HE2	1.79	0.91
1:A:480:ILE:HG22	1:A:481:THR:H	1.35	0.91
1:A:57:HIS:HB2	1:A:89:LYS:NZ	1.85	0.91
1:A:186:LYS:O	1:A:190:GLN:N	2.05	0.90
1:A:471:ARG:CG	1:A:585:TRP:CZ3	2.55	0.90
2:B:1790:ILE:HG12	2:B:1817:TRP:CZ3	2.07	0.90
2:B:1934:MET:CB	2:B:2016:VAL:HB	2.02	0.89
2:B:1983:PHE:O	2:B:1984:GLU:HB2	1.71	0.89
2:B:2264:SER:CB	2:B:2301:LEU:HD21	2.01	0.89
1:A:621:VAL:HG12	1:A:622:PHE:N	1.88	0.89
2:B:2213:GLN:HA	2:B:2217:ASN:HD22	1.38	0.89
1:A:656:TYR:CE1	2:B:1791:SER:HB2	2.08	0.89
1:A:670:LEU:HD12	1:A:671:PHE:H	1.36	0.89
1:A:105:TYR:CB	1:A:109:SER:HB3	2.02	0.88
1:A:105:TYR:CD2	1:A:110:GLU:HB3	2.08	0.88
2:B:1791:SER:O	2:B:1793:GLU:HG3	1.74	0.88
2:B:1973:MET:HE3	2:B:1976:TYR:HB2	1.54	0.88
1:A:165:VAL:HG12	1:A:206:LYS:HG2	1.54	0.88
2:B:1829:GLU:CB	2:B:1966:ARG:HD2	2.02	0.87
1:A:65:ARG:CB	1:A:66:PRO:CD	2.52	0.87
1:A:651:VAL:N	1:A:693:HIS:HB2	1.89	0.87
1:A:7:LEU:HD11	1:A:51:PHE:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ALA:HB1	1:A:397:PRO:HA	1.57	0.86
2:B:2048:PRO:HG3	2:B:2062:TRP:CD1	2.10	0.86
2:B:2096:LEU:CB	2:B:2161:THR:HG21	2.01	0.86
2:B:2245:THR:C	2:B:2286:ASN:HD21	1.78	0.86
2:B:2055:TYR:HD1	2:B:2060:ASN:ND2	1.73	0.86
1:A:617:ILE:CD1	1:A:706:LEU:HD13	2.05	0.86
2:B:2262:ILE:H	2:B:2262:ILE:HD12	1.41	0.86
1:A:625:LEU:HD11	1:A:706:LEU:HD11	1.57	0.85
1:A:656:TYR:HB2	1:A:686:GLY:HA2	1.57	0.85
2:B:1707:TRP:HE1	2:B:1758:LEU:CD2	1.88	0.85
1:A:395:TYR:HE2	1:A:614:MET:HG3	1.39	0.85
1:A:656:TYR:HB2	1:A:686:GLY:CA	2.05	0.85
2:B:1829:GLU:HB2	2:B:1966:ARG:NH1	1.92	0.85
1:A:65:ARG:CB	1:A:66:PRO:HD3	2.06	0.84
2:B:1738:PHE:CE2	2:B:1747:LEU:HD12	2.12	0.84
1:A:453:LEU:CD2	1:A:533:TYR:CE2	2.61	0.84
1:A:182:GLY:O	1:A:186:LYS:HE3	1.77	0.84
1:A:705:LEU:O	1:A:706:LEU:HB2	1.77	0.84
2:B:1786:TYR:CA	2:B:1790:ILE:HD11	2.06	0.84
2:B:1830:PHE:CE1	2:B:1966:ARG:NH1	2.45	0.84
1:A:389:GLU:OE1	1:A:429:MET:CE	2.25	0.84
1:A:448:ILE:HD13	1:A:448:ILE:H	1.42	0.83
2:B:1829:GLU:HB2	2:B:1966:ARG:CD	2.07	0.83
1:A:237:TYR:CG	1:A:242:LEU:HB3	2.13	0.83
1:A:656:TYR:OH	2:B:1792:TYR:CE1	2.29	0.83
2:B:1790:ILE:HG12	2:B:1817:TRP:HZ3	1.42	0.83
1:A:141:LEU:CD2	1:A:143:GLU:HB3	2.08	0.83
1:A:696:ASP:O	1:A:699:ASN:HB2	1.77	0.83
2:B:1786:TYR:HA	2:B:1790:ILE:HD12	1.60	0.83
2:B:2180:MET:CB	2:B:2322:GLU:OE2	2.21	0.83
1:A:485:PRO:HD3	1:A:498:LEU:HD21	1.59	0.83
2:B:1707:TRP:NE1	2:B:1758:LEU:HD23	1.92	0.83
1:A:378:HIS:HB3	1:A:379:PRO:HD2	1.59	0.83
2:B:2055:TYR:HD1	2:B:2060:ASN:HD22	1.24	0.83
1:A:541:ARG:HG2	1:A:585:TRP:HE1	1.44	0.83
2:B:1732:LYS:HG2	2:B:1849:SER:O	1.78	0.83
2:B:1738:PHE:HB3	2:B:1747:LEU:HA	1.61	0.83
1:A:281:HIS:ND1	1:A:524:SER:HB3	1.94	0.83
1:A:686:GLY:O	1:A:687:LEU:HD23	1.79	0.83
1:A:649:LEU:O	1:A:695:SER:HB3	1.77	0.82
2:B:2055:TYR:HA	2:B:2060:ASN:HB3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD22	1:A:274:HIS:HB2	1.61	0.82
1:A:471:ARG:HG2	1:A:585:TRP:HE3	1.41	0.82
2:B:2083:GLY:CA	2:B:2140:PHE:HD2	1.91	0.82
2:B:2264:SER:OG	2:B:2301:LEU:CD2	2.24	0.82
2:B:2330:ASP:HB3	2:B:2331:LEU:CD2	2.09	0.82
1:A:169:ASN:O	1:A:170:SER:OG	1.98	0.82
2:B:1947:MET:HE2	2:B:1948:GLY:N	1.91	0.82
1:A:285:SER:HB2	1:A:676:GLU:OE2	1.78	0.82
1:A:287:GLU:CB	1:A:673:PHE:CD2	2.61	0.82
2:B:2262:ILE:HD12	2:B:2262:ILE:N	1.94	0.82
1:A:428:PHE:HE1	1:A:547:LEU:HB3	1.42	0.82
1:A:615:HIS:CB	1:A:703:THR:HB	2.09	0.82
2:B:1983:PHE:HD1	2:B:1984:GLU:H	1.23	0.81
2:B:1829:GLU:CA	2:B:1966:ARG:HD2	2.10	0.81
1:A:65:ARG:HG3	1:A:66:PRO:N	1.96	0.81
2:B:1883:PHE:O	2:B:1917:ARG:HA	1.80	0.81
1:A:471:ARG:HG2	1:A:585:TRP:CZ3	2.16	0.81
2:B:1946:SER:CB	2:B:1978:LEU:HB3	2.08	0.81
1:A:471:ARG:CG	1:A:585:TRP:HZ3	1.93	0.81
2:B:1940:ILE:HD12	2:B:1990:PRO:HD3	1.63	0.81
1:A:534:SER:HB3	1:A:536:PHE:HE1	1.45	0.81
2:B:1885:GLU:O	2:B:1887:LYS:N	2.13	0.81
1:A:575:LEU:N	1:A:618:ASN:OD1	2.14	0.81
1:A:495:VAL:HG21	1:A:501:PHE:HB2	1.63	0.80
2:B:1934:MET:HB3	2:B:2016:VAL:CB	2.10	0.80
2:B:2306:LEU:HD23	2:B:2307:ARG:N	1.95	0.80
1:A:100:ALA:HB2	1:A:138:TRP:CE3	2.15	0.80
1:A:664:TYR:CE1	2:B:1826:THR:HG23	2.14	0.80
1:A:191:THR:OG1	1:A:193:HIS:ND1	2.14	0.80
2:B:1736:GLN:OE1	2:B:1747:LEU:HD21	1.81	0.80
2:B:2052:ARG:N	2:B:2163:ARG:HB3	1.96	0.80
2:B:1849:SER:OG	2:B:1888:SER:HB2	1.81	0.80
2:B:2036:GLN:NE2	2:B:2076:LEU:HD11	1.96	0.80
1:A:83:THR:HG22	1:A:140:VAL:H	1.46	0.80
2:B:1758:LEU:CD1	2:B:1922:ASN:C	2.50	0.80
2:B:1909:ASP:O	2:B:1913:LYS:CB	2.30	0.80
1:A:7:LEU:HD21	1:A:51:PHE:CD2	2.17	0.80
1:A:249:HIS:NE2	1:A:303:LEU:HD11	1.97	0.79
1:A:285:SER:CB	1:A:676:GLU:OE2	2.30	0.79
2:B:2273:LEU:CD2	2:B:2280:VAL:HG23	2.12	0.79
1:A:461:LEU:HB2	1:A:513:TRP:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1739:THR:H	2:B:1746:PRO:HG2	1.48	0.79
1:A:656:TYR:CG	1:A:686:GLY:HA2	2.17	0.79
2:B:1945:LEU:HD12	2:B:1945:LEU:H	1.47	0.79
1:A:293:PHE:CD1	2:B:1975:LEU:HD21	2.18	0.79
1:A:656:TYR:O	1:A:658:PHE:N	2.16	0.79
1:A:428:PHE:CE1	1:A:547:LEU:HB3	2.18	0.79
2:B:1982:VAL:O	2:B:1983:PHE:CD2	2.36	0.79
2:B:1829:GLU:HB2	2:B:1966:ARG:CZ	2.12	0.79
2:B:1790:ILE:HA	2:B:1817:TRP:CZ3	2.18	0.78
2:B:1952:ASN:HB3	2:B:1954:HIS:NE2	1.98	0.78
1:A:464:ILE:HG23	1:A:510:LYS:HG2	1.65	0.78
2:B:1865:PRO:O	2:B:1867:HIS:N	2.15	0.78
1:A:530:THR:OG1	1:A:679:PHE:HB3	1.82	0.78
1:A:647:ASP:OD1	2:B:1950:ASN:ND2	2.16	0.78
2:B:2081:ILE:HD12	2:B:2149:ILE:HD11	1.64	0.78
1:A:157:SER:HA	1:A:176:LEU:H	1.45	0.78
1:A:631:LEU:HD21	1:A:632:HIS:ND1	1.98	0.78
2:B:1813:LYS:CD	2:B:1814:THR:H	1.94	0.78
1:A:656:TYR:HH	2:B:1792:TYR:HE1	1.28	0.78
1:A:147:MET:HE3	2:B:1972:LYS:HE3	1.65	0.78
1:A:448:ILE:HD12	1:A:619:GLY:HA3	1.63	0.78
2:B:1886:THR:HG22	2:B:1913:LYS:NZ	1.99	0.78
2:B:1945:LEU:HG	2:B:1983:PHE:HB2	0.82	0.78
1:A:289:SER:HB3	1:A:290:PRO:CD	2.13	0.77
1:A:432:THR:HA	1:A:438:THR:OG1	1.82	0.77
2:B:1838:PHE:HZ	2:B:1947:MET:CG	1.96	0.77
1:A:526:PRO:O	1:A:679:PHE:HZ	1.67	0.77
2:B:1830:PHE:HD1	2:B:1966:ARG:HH12	0.83	0.77
1:A:100:ALA:HB2	1:A:138:TRP:HZ3	1.49	0.77
1:A:700:ARG:HH22	2:B:1844:GLU:HB3	1.49	0.77
1:A:278:VAL:HG23	1:A:279:ARG:H	1.49	0.77
2:B:1699:PHE:CG	2:B:1740:ASP:OD1	2.38	0.77
1:A:529:LEU:CD1	1:A:553:ILE:HB	2.15	0.77
2:B:1863:LEU:HB2	2:B:1870:GLN:H	1.48	0.77
2:B:1891:PHE:CD1	2:B:1892:THR:N	2.40	0.77
2:B:2046:TRP:HZ3	2:B:2059:ILE:C	1.88	0.77
1:A:278:VAL:HG12	1:A:296:ALA:HB2	1.67	0.77
2:B:2081:ILE:HG13	2:B:2144:ILE:HB	1.66	0.77
1:A:456:GLU:O	1:A:459:ASP:HB2	1.83	0.77
2:B:2042:GLN:HE21	2:B:2047:ALA:HA	1.47	0.77
2:B:2089:ALA:O	2:B:2096:LEU:HB2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1773:VAL:HG11	2:B:1785:PHE:CE1	2.20	0.76
2:B:2187:ASP:HB2	2:B:2206:SER:CB	2.16	0.76
2:B:2042:GLN:OE1	2:B:2042:GLN:N	2.17	0.76
1:A:529:LEU:HA	1:A:679:PHE:CE1	2.20	0.76
2:B:2234:PHE:HB2	2:B:2304:ARG:O	1.85	0.76
1:A:474:ASN:O	1:A:535:SER:HA	1.85	0.76
2:B:1882:ILE:HD11	2:B:1919:HIS:ND1	1.99	0.76
1:A:100:ALA:CB	1:A:138:TRP:CZ3	2.68	0.76
1:A:148:ALA:CA	1:A:180:ARG:NH2	2.49	0.76
2:B:2000:CYS:SG	2:B:2002:ILE:HD12	2.25	0.76
1:A:77:GLN:HB3	1:A:177:LEU:HD12	1.68	0.76
1:A:491:LEU:HB3	1:A:492:PRO:HD2	1.68	0.76
2:B:1751:GLU:HG3	2:B:2117:GLY:H	1.51	0.76
2:B:1789:LEU:CD2	2:B:1823:MET:HB3	2.16	0.76
2:B:1735:PHE:HE1	2:B:1851:LEU:HG	1.50	0.76
2:B:2013:LEU:HD22	2:B:2013:LEU:N	2.01	0.75
1:A:281:HIS:CE1	1:A:524:SER:HB3	2.22	0.75
1:A:613:ILE:O	1:A:613:ILE:HG13	1.85	0.75
2:B:1795:ASP:OD2	2:B:1800:ALA:HB2	1.87	0.75
1:A:382:TRP:HE1	1:A:454:TYR:HB3	1.51	0.75
1:A:622:PHE:CZ	1:A:702:MET:O	2.39	0.75
2:B:1707:TRP:CE2	2:B:1758:LEU:HD23	2.22	0.75
1:A:287:GLU:CA	1:A:673:PHE:HE2	2.00	0.74
1:A:688:TRP:CZ2	2:B:1799:GLY:HA2	2.22	0.74
2:B:2027:MET:HB3	2:B:2165:GLU:HG2	1.67	0.74
1:A:668:LEU:HG	2:B:1788:SER:OG	1.86	0.74
1:A:311:HIS:O	1:A:312:ILE:HG12	1.87	0.74
1:A:454:TYR:HE1	1:A:456:GLU:HG2	1.50	0.74
1:A:651:VAL:HG13	1:A:668:LEU:HA	1.67	0.74
2:B:1886:THR:CG2	2:B:1913:LYS:HZ1	1.99	0.74
2:B:2034:ASP:CB	2:B:2049:LYS:HD2	2.17	0.74
1:A:662:MET:HG3	1:A:680:MET:CE	2.17	0.74
1:A:385:TYR:CD2	1:A:436:PHE:O	2.40	0.74
1:A:503:ILE:O	1:A:504:LEU:HD12	1.86	0.74
1:A:393:TRP:CD1	1:A:395:TYR:HE1	2.05	0.74
1:A:105:TYR:O	1:A:106:TRP:HB2	1.86	0.74
2:B:1738:PHE:HD2	2:B:1747:LEU:CD1	1.87	0.74
1:A:306:PHE:N	1:A:306:PHE:CD1	2.40	0.73
1:A:453:LEU:HD21	1:A:533:TYR:HE2	1.49	0.73
2:B:2329:GLN:HG3	2:B:2332:TYR:C	2.09	0.73
1:A:90:ASN:OD1	1:A:92:ALA:HB3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:CE2	1:A:110:GLU:HB3	2.23	0.73
2:B:1997:ARG:HD2	2:B:2011:SER:OG	1.88	0.73
1:A:471:ARG:CG	1:A:585:TRP:CE3	2.67	0.73
1:A:480:ILE:HG22	1:A:481:THR:N	2.03	0.73
1:A:471:ARG:HG3	1:A:585:TRP:HZ3	1.53	0.73
1:A:617:ILE:HD11	1:A:705:LEU:O	1.88	0.73
2:B:1964:THR:O	2:B:1986:VAL:CG1	2.36	0.73
1:A:148:ALA:HA	1:A:180:ARG:HH22	1.53	0.73
2:B:1889:TRP:HA	2:B:1889:TRP:CE3	2.22	0.73
1:A:123:LYS:HA	1:A:126:ASP:HB2	1.69	0.73
1:A:389:GLU:OE1	1:A:431:TYR:CZ	2.42	0.72
1:A:491:LEU:C	1:A:493:LYS:H	1.91	0.72
1:A:495:VAL:HG22	1:A:496:LYS:N	2.04	0.72
2:B:1759:LEU:HD22	2:B:1854:PRO:HG3	1.71	0.72
2:B:1891:PHE:HD1	2:B:1892:THR:H	0.80	0.72
2:B:2081:ILE:HA	2:B:2168:GLY:HA3	1.71	0.72
1:A:412:LEU:HA	1:A:420:GLY:HA3	1.72	0.72
1:A:65:ARG:HG3	1:A:66:PRO:CD	2.17	0.72
1:A:114:TYR:O	1:A:116:ASP:N	2.22	0.72
1:A:653:PHE:HB2	1:A:693:HIS:HE1	1.55	0.72
1:A:664:TYR:CD1	2:B:1826:THR:HG23	2.25	0.72
1:A:697:PHE:CG	1:A:698:ARG:N	2.58	0.72
1:A:416:PRO:HA	1:A:596:PRO:HG3	1.71	0.72
2:B:1947:MET:CE	2:B:1948:GLY:N	2.47	0.72
2:B:1997:ARG:HG2	2:B:1999:GLU:HG3	1.72	0.72
2:B:2032:ILE:CG2	2:B:2036:GLN:OE1	2.30	0.72
1:A:624:SER:C	1:A:625:LEU:HD12	2.10	0.72
2:B:2036:GLN:HG2	2:B:2076:LEU:HD21	1.71	0.72
1:A:700:ARG:NH1	2:B:1843:LEU:HB3	2.05	0.72
2:B:1830:PHE:HD2	2:B:1985:THR:HG1	1.34	0.72
1:A:50:LEU:HB3	1:A:171:GLY:HA3	1.72	0.71
1:A:663:VAL:HG13	2:B:1968:LYS:HB2	1.72	0.71
1:A:375:ALA:C	1:A:376:LYS:HG2	2.10	0.71
2:B:1758:LEU:HD11	2:B:1922:ASN:C	2.10	0.71
1:A:473:TYR:CD2	1:A:547:LEU:HD11	2.25	0.71
1:A:651:VAL:CG1	1:A:668:LEU:HA	2.19	0.71
2:B:1963:PHE:CG	2:B:1986:VAL:HG11	2.24	0.71
1:A:375:ALA:O	1:A:376:LYS:HG2	1.90	0.71
1:A:616:SER:O	1:A:620:TYR:N	2.21	0.71
2:B:1707:TRP:HA	2:B:1707:TRP:CE3	2.26	0.71
2:B:2097:TYR:CZ	2:B:2157:SER:OG	2.41	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HB3	1:A:136:TYR:CZ	2.25	0.71
2:B:1934:MET:HE3	2:B:1940:ILE:CD1	2.10	0.71
1:A:605:ASP:O	1:A:609:GLN:HG3	1.91	0.71
2:B:2055:TYR:CD1	2:B:2060:ASN:ND2	2.55	0.71
2:B:2273:LEU:CD2	2:B:2280:VAL:HG21	2.12	0.71
1:A:4:ARG:HG3	1:A:85:VAL:HG23	1.71	0.71
1:A:420:GLY:O	1:A:421:ARG:HG2	1.91	0.71
2:B:1789:LEU:N	2:B:1789:LEU:HD12	2.06	0.71
2:B:1878:LEU:HA	2:B:1922:ASN:HD21	1.55	0.71
2:B:2087:GLN:HG2	2:B:2163:ARG:CD	2.20	0.71
2:B:2149:ILE:HD12	2:B:2166:LEU:HD22	1.72	0.71
1:A:667:THR:O	1:A:669:THR:N	2.24	0.71
1:A:667:THR:OG1	1:A:668:LEU:N	2.24	0.71
2:B:2264:SER:HB3	2:B:2301:LEU:CD2	2.21	0.70
1:A:428:PHE:HE2	1:A:475:ILE:HG12	1.55	0.70
1:A:663:VAL:CG1	2:B:1968:LYS:HB2	2.21	0.70
2:B:1786:TYR:CA	2:B:1790:ILE:CD1	2.58	0.70
2:B:1819:VAL:HA	2:B:1823:MET:CE	2.21	0.70
2:B:1945:LEU:HA	2:B:1983:PHE:CA	2.15	0.70
5:E:3:BMA:O3	5:E:5:MAN:C1	2.39	0.70
1:A:646:THR:OG1	2:B:1950:ASN:OD1	2.09	0.70
1:A:522:THR:N	1:A:525:ASP:OD1	2.24	0.70
2:B:1735:PHE:HE1	2:B:1851:LEU:CG	2.04	0.70
1:A:412:LEU:HA	1:A:420:GLY:CA	2.21	0.70
1:A:287:GLU:HG2	1:A:673:PHE:HD2	1.57	0.70
2:B:1743:PHE:CE1	2:B:1778:GLN:CD	2.57	0.70
2:B:1948:GLY:HA3	2:B:1952:ASN:HD21	1.57	0.70
2:B:2051:ALA:HA	2:B:2163:ARG:HA	1.73	0.70
2:B:1731:LYS:H	2:B:1893:GLU:CD	1.96	0.70
1:A:147:MET:O	1:A:148:ALA:HB3	1.91	0.70
1:A:651:VAL:HB	1:A:693:HIS:CE1	2.26	0.70
1:A:287:GLU:CG	1:A:673:PHE:CD2	2.75	0.69
2:B:1758:LEU:HD12	2:B:1922:ASN:C	2.12	0.69
1:A:534:SER:HB3	1:A:536:PHE:CE1	2.27	0.69
2:B:2306:LEU:CD2	2:B:2307:ARG:N	2.55	0.69
2:B:1997:ARG:CD	2:B:2011:SER:OG	2.41	0.69
1:A:147:MET:CE	2:B:1972:LYS:HE3	2.21	0.69
2:B:1763:ILE:HG23	2:B:1855:LEU:HG	1.73	0.69
1:A:616:SER:O	1:A:617:ILE:HG22	1.93	0.69
2:B:1834:ALA:O	2:B:1945:LEU:HD21	1.91	0.69
2:B:2034:ASP:HB3	2:B:2049:LYS:CD	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1945:LEU:H	2:B:1945:LEU:CD1	2.05	0.69
2:B:1838:PHE:CZ	2:B:1947:MET:CG	2.75	0.69
1:A:287:GLU:CG	1:A:673:PHE:HD2	2.05	0.69
1:A:395:TYR:CE2	1:A:614:MET:HG3	2.26	0.69
1:A:486:LEU:O	1:A:487:TYR:HB2	1.92	0.69
1:A:7:LEU:HD12	1:A:52:VAL:O	1.91	0.68
1:A:249:HIS:CD2	1:A:303:LEU:HD11	2.27	0.68
1:A:289:SER:HB3	1:A:290:PRO:HD2	1.73	0.68
1:A:454:TYR:CE1	1:A:456:GLU:HG2	2.28	0.68
1:A:687:LEU:HD12	2:B:1795:ASP:OD2	1.93	0.68
2:B:1849:SER:CB	2:B:1888:SER:HB2	2.23	0.68
2:B:1934:MET:HE3	2:B:1940:ILE:HG21	1.74	0.68
1:A:495:VAL:HG22	1:A:496:LYS:H	1.58	0.68
2:B:1963:PHE:HB2	2:B:1986:VAL:CG1	2.23	0.68
1:A:127:LYS:HG3	1:A:162:VAL:HG11	1.74	0.68
1:A:272:GLU:HB3	1:A:306:PHE:HB3	1.73	0.68
1:A:281:HIS:HB3	1:A:525:ASP:HB3	1.73	0.68
1:A:396:ALA:HB1	1:A:397:PRO:CA	2.23	0.68
2:B:2273:LEU:O	2:B:2275:PHE:CD1	2.47	0.68
2:B:1889:TRP:HA	2:B:1889:TRP:HE3	1.57	0.68
1:A:147:MET:HE2	2:B:1972:LYS:HB2	1.75	0.68
1:A:432:THR:OG1	1:A:440:GLU:CB	2.40	0.68
1:A:587:LEU:O	1:A:591:ILE:HG22	1.94	0.68
1:A:684:ASN:O	1:A:686:GLY:N	2.23	0.68
2:B:1776:ARG:HG2	2:B:1812:THR:HG22	1.76	0.68
1:A:65:ARG:HB3	1:A:66:PRO:CD	2.23	0.68
2:B:1831:ASP:O	2:B:1858:CYS:HB3	1.94	0.68
2:B:1838:PHE:CZ	2:B:1947:MET:SD	2.87	0.68
2:B:1942:TRP:HB3	2:B:1944:LEU:HD21	1.75	0.68
1:A:57:HIS:HB2	1:A:89:LYS:HZ1	1.59	0.68
1:A:428:PHE:HE2	1:A:475:ILE:CG1	2.06	0.68
1:A:457:VAL:CG1	1:A:517:VAL:HA	2.24	0.68
1:A:57:HIS:O	1:A:58:LEU:HG	1.94	0.67
1:A:141:LEU:HD22	1:A:143:GLU:HB3	1.75	0.67
1:A:480:ILE:CG2	1:A:481:THR:H	2.06	0.67
1:A:642:ILE:HG22	1:A:643:GLY:N	2.06	0.67
2:B:2262:ILE:HD11	2:B:2283:PHE:CE1	2.28	0.67
3:C:3:BMA:H61	3:C:4:MAN:C3	2.13	0.67
1:A:97:SER:O	1:A:160:SER:HB3	1.94	0.67
1:A:605:ASP:OD2	1:A:607:GLU:HB3	1.93	0.67
2:B:2042:GLN:HB3	2:B:2062:TRP:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:NAG:O3	3:C:3:BMA:O5	2.11	0.67
1:A:696:ASP:O	1:A:699:ASN:CB	2.42	0.67
2:B:2273:LEU:O	2:B:2275:PHE:CE1	2.48	0.67
1:A:389:GLU:OE1	1:A:429:MET:HE1	1.95	0.67
1:A:581:GLU:HB2	1:A:612:ASN:O	1.95	0.67
1:A:617:ILE:HG12	1:A:706:LEU:CD2	2.25	0.67
1:A:700:ARG:CZ	2:B:1844:GLU:HB2	2.24	0.67
1:A:477:PRO:HG3	1:A:513:TRP:CE2	2.29	0.67
2:B:1784:SER:O	2:B:1839:SER:HA	1.94	0.67
2:B:2096:LEU:HD12	2:B:2159:ARG:HB3	1.77	0.67
1:A:72:LEU:HG	1:A:198:LEU:HD12	1.76	0.67
1:A:538:ASN:HD21	1:A:541:ARG:HB3	1.60	0.67
1:A:428:PHE:CE2	1:A:475:ILE:HG12	2.30	0.67
2:B:2249:LYS:HE3	2:B:2249:LYS:H	1.59	0.67
1:A:700:ARG:NH1	2:B:1844:GLU:HB2	2.10	0.67
1:A:270:PHE:HB2	1:A:309:PHE:HE1	1.59	0.66
1:A:448:ILE:HD13	1:A:448:ILE:N	2.10	0.66
1:A:640:LEU:CB	1:A:677:THR:HB	2.25	0.66
2:B:1837:TYR:CZ	2:B:1853:GLY:HA3	2.30	0.66
2:B:1943:TYR:C	2:B:1944:LEU:HD23	2.15	0.66
2:B:2087:GLN:HG2	2:B:2163:ARG:HD3	1.75	0.66
1:A:94:HIS:HB3	1:A:96:VAL:HG13	1.77	0.66
2:B:1735:PHE:CE1	2:B:1851:LEU:HB2	2.30	0.66
2:B:1819:VAL:HA	2:B:1823:MET:HE2	1.75	0.66
2:B:1849:SER:OG	2:B:1888:SER:CB	2.42	0.66
2:B:1945:LEU:CA	2:B:1983:PHE:HA	2.15	0.66
1:A:457:VAL:HG11	1:A:517:VAL:HA	1.76	0.66
1:A:687:LEU:CD1	2:B:1795:ASP:OD2	2.43	0.66
1:A:700:ARG:HH12	2:B:1844:GLU:HB2	1.59	0.66
2:B:1946:SER:HB2	2:B:1978:LEU:HD12	1.74	0.66
2:B:2036:GLN:HE21	2:B:2076:LEU:HD11	1.59	0.66
1:A:448:ILE:CD1	1:A:618:ASN:O	2.44	0.66
1:A:577:SER:O	1:A:616:SER:HB3	1.96	0.66
2:B:2022:GLN:HG3	2:B:2082:HIS:ND1	2.10	0.66
2:B:2031:HIS:HB2	2:B:2294:VAL:HG11	1.78	0.66
1:A:147:MET:HE3	2:B:1972:LYS:CE	2.26	0.66
2:B:2027:MET:CE	2:B:2032:ILE:HD13	2.25	0.66
1:A:272:GLU:HB2	1:A:307:LEU:H	1.60	0.66
1:A:473:TYR:HA	1:A:537:VAL:CG2	2.25	0.66
1:A:697:PHE:CE1	1:A:698:ARG:HB2	2.31	0.66
1:A:80:VAL:HA	1:A:140:VAL:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1774:THR:HG22	2:B:1814:THR:CG2	2.25	0.66
2:B:2331:LEU:O	2:B:2332:TYR:HB2	1.95	0.66
1:A:651:VAL:HB	1:A:693:HIS:ND1	2.11	0.65
1:A:475:ILE:HG23	1:A:475:ILE:O	1.97	0.65
1:A:657:THR:O	1:A:658:PHE:HB2	1.94	0.65
1:A:114:TYR:CE2	2:B:1997:ARG:HD3	2.31	0.65
1:A:293:PHE:HD1	2:B:1975:LEU:HD21	1.58	0.65
1:A:664:TYR:OH	2:B:1825:PRO:HA	1.95	0.65
1:A:670:LEU:HG	1:A:672:PRO:HD3	1.79	0.65
2:B:1997:ARG:HG2	2:B:1999:GLU:CG	2.26	0.65
2:B:2129:ASN:HB3	2:B:2134:GLY:HA3	1.78	0.65
1:A:398:LEU:CD2	1:A:399:VAL:HG12	2.23	0.65
1:A:417:GLN:O	1:A:418:ARG:HG2	1.97	0.65
1:A:542:ASP:O	1:A:545:SER:N	2.29	0.65
1:A:623:ASP:OD1	1:A:705:LEU:CB	2.45	0.65
2:B:1749:ARG:HG2	2:B:1749:ARG:HH11	1.62	0.65
2:B:2220:ARG:HH11	2:B:2220:ARG:HB2	1.62	0.65
1:A:87:THR:HG22	1:A:135:THR:CB	2.27	0.65
1:A:473:TYR:HA	1:A:537:VAL:HG22	1.79	0.65
1:A:234:VAL:HG23	1:A:320:MET:HA	1.79	0.65
1:A:417:GLN:HE22	1:A:602:GLN:HB2	1.62	0.65
1:A:656:TYR:CB	1:A:686:GLY:CA	2.67	0.65
2:B:1738:PHE:CE2	2:B:1747:LEU:CD1	2.79	0.65
1:A:278:VAL:HG23	1:A:279:ARG:N	2.10	0.64
2:B:1735:PHE:CD1	2:B:1851:LEU:HB2	2.31	0.64
1:A:390:GLU:OE2	1:A:470:SER:HB2	1.96	0.64
1:A:378:HIS:HB3	1:A:379:PRO:CD	2.25	0.64
1:A:530:THR:O	1:A:531:ARG:NE	2.31	0.64
1:A:486:LEU:HD22	1:A:487:TYR:CG	2.32	0.64
1:A:617:ILE:HG12	1:A:706:LEU:HD22	1.80	0.64
1:A:292:THR:HG23	2:B:1977:ASN:HD21	1.61	0.64
2:B:1947:MET:HE3	2:B:1948:GLY:H	1.62	0.64
2:B:2276:GLN:N	2:B:2279:LYS:O	2.28	0.64
1:A:116:ASP:OD1	1:A:118:THR:HG22	1.98	0.64
2:B:2051:ALA:HB1	2:B:2164:MET:N	2.10	0.64
1:A:166:LYS:O	1:A:207:SER:HB2	1.98	0.64
1:A:686:GLY:O	1:A:687:LEU:CD2	2.45	0.64
1:A:654:SER:HB2	1:A:690:LEU:HB2	1.80	0.64
1:A:688:TRP:HE1	2:B:1799:GLY:C	2.01	0.64
2:B:2054:HIS:O	2:B:2060:ASN:CB	2.45	0.64
2:B:2263:SER:HB2	2:B:2307:ARG:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HG3	1:A:121:ARG:HH11	1.63	0.64
1:A:271:LEU:HD22	1:A:274:HIS:CB	2.27	0.64
2:B:1829:GLU:HB2	2:B:1966:ARG:NE	2.13	0.64
2:B:2105:TYR:CD2	2:B:2144:ILE:HG23	2.33	0.64
2:B:1787:SER:OG	2:B:1788:SER:N	2.30	0.63
2:B:1837:TYR:CE2	2:B:1853:GLY:HA3	2.34	0.63
2:B:1976:TYR:CE2	2:B:1984:GLU:OE2	2.50	0.63
1:A:271:LEU:HD11	1:A:324:VAL:HG11	1.80	0.63
2:B:1743:PHE:CZ	2:B:1778:GLN:NE2	2.65	0.63
2:B:2046:TRP:CZ3	2:B:2060:ASN:N	2.51	0.63
1:A:448:ILE:H	1:A:448:ILE:CD1	2.10	0.63
2:B:2080:ILE:HG12	2:B:2170:ASP:O	1.98	0.63
2:B:1758:LEU:CD1	2:B:1923:GLY:N	2.54	0.63
2:B:1953:ILE:HD12	2:B:1953:ILE:H	1.63	0.63
2:B:1934:MET:HE3	2:B:1940:ILE:CG1	2.27	0.63
1:A:509:PHE:HD1	1:A:510:LYS:H	1.47	0.63
2:B:2052:ARG:H	2:B:2163:ARG:CB	2.07	0.63
1:A:623:ASP:OD1	1:A:705:LEU:HB2	1.98	0.63
2:B:1939:ARG:NH2	2:B:1987:GLU:OE1	2.21	0.63
2:B:1889:TRP:CZ3	2:B:1890:TYR:HB2	2.34	0.62
2:B:2178:LEU:HD12	2:B:2323:VAL:HB	1.80	0.62
1:A:271:LEU:CD2	1:A:274:HIS:HB2	2.28	0.62
1:A:153:CYS:N	1:A:179:CYS:SG	2.58	0.62
2:B:2115:TYR:CE2	2:B:2140:PHE:HD1	2.17	0.62
2:B:2207:LYS:HD2	2:B:2216:SER:O	1.99	0.62
1:A:453:LEU:HD22	1:A:453:LEU:H	1.63	0.62
1:A:651:VAL:HG12	1:A:652:PHE:N	2.15	0.62
2:B:2042:GLN:HE21	2:B:2047:ALA:CA	2.12	0.62
2:B:2283:PHE:HD2	2:B:2295:ASN:HD22	1.47	0.62
1:A:656:TYR:CE2	2:B:1791:SER:HB2	2.35	0.62
2:B:2330:ASP:CB	2:B:2331:LEU:HD23	2.21	0.62
1:A:453:LEU:HD22	1:A:453:LEU:N	2.15	0.62
2:B:1963:PHE:HB2	2:B:1986:VAL:HG12	1.81	0.62
1:A:457:VAL:HG11	1:A:517:VAL:HG23	1.81	0.62
2:B:2193:SER:HA	2:B:2229:TRP:CZ2	2.34	0.62
1:A:512:LYS:HE3	1:A:514:THR:OG1	2.00	0.61
2:B:1929:LEU:HB3	2:B:2012:THR:OG1	2.00	0.61
2:B:2087:GLN:HG2	2:B:2163:ARG:NE	2.15	0.61
1:A:651:VAL:HB	1:A:693:HIS:CG	2.35	0.61
2:B:1705:ARG:HG2	2:B:1706:LEU:H	1.64	0.61
2:B:1758:LEU:CD1	2:B:1922:ASN:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1840:ASP:O	2:B:1841:VAL:HG23	1.99	0.61
1:A:56:ASP:O	1:A:57:HIS:HB3	2.00	0.61
1:A:473:TYR:O	1:A:504:LEU:CD1	2.49	0.61
1:A:529:LEU:HA	1:A:679:PHE:CD1	2.34	0.61
1:A:625:LEU:HD13	1:A:706:LEU:CD2	2.30	0.61
1:A:693:HIS:HB3	1:A:695:SER:HB2	1.81	0.61
2:B:1829:GLU:HB2	2:B:1966:ARG:HH11	1.63	0.61
1:A:282:ARG:HH12	1:A:299:LEU:HD22	1.65	0.61
2:B:1952:ASN:OD1	2:B:1952:ASN:N	2.32	0.61
2:B:2087:GLN:CG	2:B:2163:ARG:HD3	2.30	0.61
1:A:2:THR:OG1	1:A:83:THR:O	2.18	0.61
1:A:507:GLU:HG3	1:A:508:ILE:H	1.65	0.61
1:A:664:TYR:HE1	2:B:1826:THR:HG23	1.64	0.61
2:B:1732:LYS:HE3	2:B:1885:GLU:OE2	2.00	0.61
1:A:87:THR:HG22	1:A:135:THR:HB	1.83	0.61
1:A:615:HIS:HB2	1:A:703:THR:OG1	2.01	0.61
2:B:2193:SER:HB3	2:B:2229:TRP:CD1	2.35	0.61
1:A:291:ILE:HG23	2:B:1955:SER:CB	2.31	0.61
2:B:2083:GLY:CA	2:B:2140:PHE:CD2	2.72	0.61
1:A:85:VAL:HG12	1:A:137:VAL:HA	1.82	0.61
1:A:631:LEU:HD23	1:A:632:HIS:HB2	1.83	0.61
2:B:2052:ARG:HD2	2:B:2165:GLU:HB2	1.78	0.61
1:A:308:LEU:O	1:A:309:PHE:HB3	2.00	0.61
1:A:624:SER:HB2	1:A:625:LEU:HD12	1.83	0.61
2:B:1951:GLU:O	2:B:1953:ILE:HD12	2.00	0.61
1:A:287:GLU:CA	1:A:673:PHE:CE2	2.80	0.60
1:A:395:TYR:HB2	1:A:621:VAL:CG2	2.11	0.60
2:B:1934:MET:O	2:B:1935:ALA:HB3	2.00	0.60
2:B:2087:GLN:CG	2:B:2163:ARG:HB2	2.31	0.60
1:A:664:TYR:HE1	2:B:1826:THR:H	1.46	0.60
2:B:2024:PRO:HA	2:B:2167:MET:HG2	1.84	0.60
2:B:1829:GLU:CB	2:B:1966:ARG:NH1	2.64	0.60
2:B:1856:LEU:HD13	2:B:1943:TYR:CE2	2.37	0.60
2:B:1997:ARG:HD2	2:B:2011:SER:HG	1.67	0.60
1:A:697:PHE:CD1	1:A:698:ARG:N	2.57	0.60
2:B:2180:MET:H	2:B:2185:ILE:HB	1.67	0.60
2:B:2238:MET:HE3	2:B:2326:CYS:O	2.01	0.60
1:A:694:ASN:ND2	1:A:703:THR:O	2.34	0.60
1:A:237:TYR:CD2	1:A:242:LEU:HB3	2.36	0.60
1:A:660:HIS:ND1	1:A:680:MET:HE3	2.17	0.60
1:A:688:TRP:NE1	2:B:1800:ALA:N	2.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1912:PHE:O	2:B:1915:ASN:HB2	2.02	0.60
2:B:1962:VAL:HG12	2:B:1974:ALA:HB2	1.83	0.60
2:B:2302:LEU:O	2:B:2302:LEU:HD23	2.01	0.60
1:A:112:ALA:O	1:A:126:ASP:HB3	2.01	0.60
1:A:625:LEU:HD12	1:A:706:LEU:CD1	2.31	0.60
2:B:1767:VAL:O	2:B:1768:GLU:HB2	2.01	0.60
2:B:1774:THR:HG22	2:B:1814:THR:HG22	1.83	0.60
2:B:1875:GLU:OE1	2:B:1943:TYR:OH	2.18	0.60
2:B:2023:THR:HB	2:B:2176:MET:HE3	1.84	0.60
1:A:312:ILE:HD12	1:A:315:HIS:ND1	2.17	0.60
1:A:393:TRP:CD1	1:A:395:TYR:CE1	2.90	0.60
2:B:1870:GLN:OE1	2:B:1872:THR:N	2.31	0.60
2:B:1945:LEU:HD12	2:B:1945:LEU:N	2.17	0.60
1:A:10:VAL:CG2	1:A:52:VAL:HG21	2.30	0.59
1:A:237:TYR:CE1	1:A:242:LEU:HB2	2.36	0.59
1:A:398:LEU:O	1:A:400:LEU:HD23	2.02	0.59
2:B:1735:PHE:CE1	2:B:1851:LEU:HD23	2.36	0.59
1:A:657:THR:HB	2:B:1788:SER:O	2.01	0.59
2:B:1842:ASP:O	2:B:1846:ASP:OD1	2.20	0.59
1:A:658:PHE:CZ	1:A:684:ASN:ND2	2.70	0.59
2:B:1842:ASP:HB2	2:B:1846:ASP:OD2	2.01	0.59
1:A:620:TYR:C	1:A:621:VAL:HG23	2.22	0.59
1:A:8:GLY:HA3	1:A:52:VAL:CG2	2.32	0.59
1:A:72:LEU:HD11	1:A:198:LEU:HB2	1.85	0.59
1:A:147:MET:O	1:A:148:ALA:CB	2.49	0.59
2:B:1787:SER:H	2:B:1790:ILE:CD1	2.15	0.59
1:A:529:LEU:HD11	1:A:553:ILE:HB	1.84	0.59
1:A:155:THR:HG22	1:A:256:HIS:ND1	2.17	0.59
1:A:483:VAL:HG13	1:A:513:TRP:HD1	1.67	0.59
1:A:495:VAL:CG2	1:A:496:LYS:H	2.16	0.59
1:A:623:ASP:OD1	1:A:705:LEU:HG	2.03	0.59
2:B:2213:GLN:HA	2:B:2217:ASN:ND2	2.12	0.59
1:A:386:ILE:HD11	1:A:428:PHE:HD2	1.68	0.59
1:A:685:PRO:HG2	2:B:1822:HIS:HE1	1.68	0.59
1:A:688:TRP:CE2	2:B:1799:GLY:HA2	2.38	0.59
1:A:393:TRP:O	1:A:422:LYS:HA	2.02	0.59
2:B:1849:SER:CA	2:B:1888:SER:HB2	2.33	0.59
1:A:395:TYR:CB	1:A:621:VAL:HG23	1.97	0.59
1:A:624:SER:HB2	1:A:625:LEU:CD1	2.33	0.59
2:B:1989:LEU:HG	2:B:1989:LEU:O	2.03	0.59
1:A:498:LEU:O	1:A:502:PRO:HD2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1735:PHE:CE1	2:B:1851:LEU:CG	2.85	0.58
2:B:1976:TYR:HE2	2:B:1984:GLU:OE1	1.86	0.58
2:B:2220:ARG:HH11	2:B:2220:ARG:CB	2.16	0.58
2:B:1836:ALA:HB2	2:B:1945:LEU:HD23	1.84	0.58
2:B:1934:MET:O	2:B:1935:ALA:CB	2.51	0.58
1:A:423:TYR:CE2	1:A:581:GLU:HG3	2.39	0.58
1:A:382:TRP:CD1	1:A:454:TYR:O	2.57	0.58
2:B:2198:ASN:OD1	2:B:2199:MET:N	2.36	0.58
1:A:141:LEU:HD23	1:A:143:GLU:N	2.06	0.58
1:A:263:THR:OG1	1:A:264:PRO:HD2	2.03	0.58
1:A:5:TYR:HE2	1:A:76:ILE:CB	1.99	0.58
1:A:147:MET:CE	2:B:1972:LYS:CE	2.81	0.58
2:B:1789:LEU:HD12	2:B:1789:LEU:H	1.66	0.58
1:A:305:GLN:C	1:A:306:PHE:HD1	2.07	0.58
1:A:509:PHE:HB3	1:A:511:TYR:HE1	1.69	0.58
2:B:1813:LYS:CD	2:B:1814:THR:N	2.54	0.58
1:A:242:LEU:HD12	1:A:243:PRO:O	2.04	0.58
1:A:652:PHE:O	1:A:657:THR:O	2.22	0.58
2:B:2248:VAL:O	2:B:2255:MET:HG2	2.03	0.58
2:B:2273:LEU:HD22	2:B:2280:VAL:HB	1.85	0.58
2:B:1925:ILE:O	2:B:1928:THR:OG1	2.22	0.58
2:B:2084:ILE:HD11	2:B:2164:MET:SD	2.44	0.58
2:B:2265:SER:HB3	2:B:2267:ASP:H	1.68	0.58
1:A:79:GLU:HG3	1:A:82:ASP:HB2	1.85	0.57
1:A:658:PHE:C	1:A:659:LYS:HD3	2.24	0.57
2:B:1952:ASN:HB3	2:B:1954:HIS:HE2	1.69	0.57
2:B:2102:ILE:HG21	2:B:2123:LEU:HD22	1.85	0.57
1:A:688:TRP:HE1	2:B:1800:ALA:H	1.50	0.57
5:E:2:NAG:H61	5:E:3:BMA:H2	1.84	0.57
1:A:292:THR:HG23	2:B:1977:ASN:ND2	2.19	0.57
1:A:313:SER:O	1:A:316:GLN:NE2	2.37	0.57
2:B:1863:LEU:CB	2:B:1870:GLN:H	2.14	0.57
2:B:1755:HIS:CD2	2:B:1876:PHE:HD1	2.21	0.57
2:B:1983:PHE:CG	2:B:1984:GLU:N	2.72	0.57
1:A:693:HIS:CD2	1:A:695:SER:HB2	2.40	0.57
2:B:1977:ASN:N	2:B:1977:ASN:OD1	2.36	0.57
1:A:191:THR:OG1	1:A:193:HIS:CG	2.58	0.57
1:A:657:THR:HG1	2:B:1786:TYR:HE2	1.49	0.57
2:B:1755:HIS:HB3	2:B:1931:GLY:O	2.04	0.57
1:A:10:VAL:HG23	1:A:52:VAL:CG2	2.31	0.57
1:A:147:MET:HE3	2:B:1972:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:SER:HA	1:A:176:LEU:N	2.18	0.57
1:A:409:SER:OG	1:A:413:ASN:OD1	2.12	0.57
1:A:432:THR:HB	1:A:433:ASP:OD1	2.04	0.57
1:A:471:ARG:HB3	1:A:585:TRP:CZ3	2.40	0.57
2:B:1840:ASP:O	2:B:1841:VAL:CB	2.52	0.57
2:B:1979:TYR:O	2:B:1980:PRO:C	2.41	0.57
1:A:492:PRO:HG2	1:A:495:VAL:HG12	1.87	0.57
2:B:1756:LEU:N	2:B:1756:LEU:HD23	2.19	0.57
2:B:2061:ALA:HB2	2:B:2163:ARG:HG3	1.86	0.57
1:A:401:ALA:HB1	1:A:405:ARG:HG3	1.86	0.57
2:B:2030:GLY:HA3	2:B:2293:VAL:HG23	1.87	0.57
2:B:2105:TYR:HA	2:B:2148:TYR:O	2.05	0.57
1:A:57:HIS:CB	1:A:89:LYS:NZ	2.64	0.56
1:A:197:LEU:HD12	1:A:255:TRP:HB3	1.87	0.56
1:A:642:ILE:CG2	1:A:643:GLY:H	2.12	0.56
2:B:1763:ILE:HG23	2:B:1763:ILE:O	2.05	0.56
1:A:65:ARG:CG	1:A:66:PRO:N	2.61	0.56
1:A:97:SER:O	1:A:160:SER:CB	2.54	0.56
1:A:577:SER:O	1:A:616:SER:CB	2.53	0.56
1:A:617:ILE:O	1:A:618:ASN:CB	2.41	0.56
2:B:2072:LYS:HA	2:B:2150:ARG:HA	1.86	0.56
1:A:49:THR:H	1:A:170:SER:HB2	1.71	0.56
1:A:184:LEU:HD23	1:A:187:GLU:HB3	1.86	0.56
1:A:453:LEU:HD21	1:A:533:TYR:CD2	2.37	0.56
1:A:483:VAL:HG13	1:A:513:TRP:CD1	2.40	0.56
1:A:625:LEU:CD1	1:A:706:LEU:HG	2.29	0.56
2:B:1781:ARG:O	2:B:1781:ARG:HG3	2.04	0.56
2:B:1948:GLY:HA3	2:B:1952:ASN:ND2	2.21	0.56
2:B:2021:CYS:O	2:B:2169:CYS:SG	2.63	0.56
1:A:279:ARG:O	1:A:280:ASN:HB3	2.06	0.56
1:A:667:THR:HG23	1:A:668:LEU:HD12	1.88	0.56
2:B:1786:TYR:CA	2:B:1790:ILE:HD12	2.32	0.56
2:B:1940:ILE:CD1	2:B:1990:PRO:HD3	2.35	0.56
2:B:2043:TYR:HB3	2:B:2065:LYS:HG2	1.86	0.56
2:B:2170:ASP:OD1	2:B:2171:LEU:HD12	2.05	0.56
2:B:1749:ARG:HG2	2:B:1749:ARG:NH1	2.21	0.56
1:A:417:GLN:C	1:A:418:ARG:HG2	2.26	0.56
1:A:645:GLN:CD	1:A:645:GLN:H	2.09	0.56
2:B:2200:PHE:CE1	2:B:2215:ARG:HD3	2.40	0.56
2:B:2264:SER:HG	2:B:2301:LEU:HD21	1.64	0.56
1:A:453:LEU:O	1:A:551:LEU:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:LEU:HB3	1:A:677:THR:HB	1.86	0.56
2:B:1709:TYR:CE2	2:B:1924:TYR:HA	2.41	0.56
2:B:1732:LYS:CG	2:B:1849:SER:O	2.51	0.56
2:B:1918:PHE:HA	2:B:1925:ILE:HD12	1.86	0.56
1:A:302:ASP:C	1:A:303:LEU:HD12	2.26	0.56
2:B:2027:MET:HE2	2:B:2032:ILE:HG21	1.88	0.56
2:B:2097:TYR:CE1	2:B:2157:SER:OG	2.58	0.56
1:A:648:PHE:O	1:A:671:PHE:HA	2.05	0.56
2:B:1764:ARG:NH1	2:B:1875:GLU:OE2	2.38	0.56
2:B:1946:SER:HB3	2:B:1978:LEU:CB	2.31	0.56
2:B:2233:ASP:HA	2:B:2305:TYR:CD1	2.41	0.56
1:A:448:ILE:HD13	1:A:618:ASN:O	2.06	0.55
1:A:72:LEU:HD13	1:A:235:ASN:OD1	2.06	0.55
1:A:633:GLU:O	1:A:684:ASN:HB2	2.06	0.55
2:B:1946:SER:CB	2:B:1978:LEU:CD1	2.63	0.55
2:B:2013:LEU:HD22	2:B:2013:LEU:H	1.70	0.55
2:B:2042:GLN:HG3	2:B:2047:ALA:HA	1.88	0.55
1:A:278:VAL:CG1	1:A:296:ALA:HB2	2.35	0.55
1:A:384:HIS:HB3	1:A:386:ILE:CG2	2.36	0.55
2:B:1694:LYS:HG3	2:B:1769:ASP:HB3	1.89	0.55
2:B:1829:GLU:CB	2:B:1966:ARG:CD	2.75	0.55
2:B:1865:PRO:C	2:B:1867:HIS:H	2.07	0.55
1:A:389:GLU:OE1	1:A:429:MET:HE3	2.06	0.55
1:A:457:VAL:HA	1:A:515:VAL:CG1	2.37	0.55
1:A:622:PHE:CE1	1:A:702:MET:C	2.78	0.55
2:B:1826:THR:OG1	2:B:1828:ASP:HB2	2.07	0.55
2:B:1934:MET:CG	2:B:2016:VAL:HB	2.37	0.55
1:A:147:MET:CE	2:B:1972:LYS:HB2	2.36	0.55
1:A:625:LEU:HD13	1:A:706:LEU:HD11	1.53	0.55
1:A:656:TYR:CZ	2:B:1791:SER:CB	2.84	0.55
2:B:1739:THR:HB	2:B:1746:PRO:CG	2.36	0.55
2:B:2259:GLU:HB2	2:B:2312:SER:H	1.70	0.55
1:A:307:LEU:HD12	1:A:322:ALA:O	2.06	0.55
1:A:418:ARG:HH21	1:A:607:GLU:HG2	1.72	0.55
1:A:471:ARG:CB	1:A:585:TRP:CZ3	2.90	0.55
1:A:538:ASN:ND2	1:A:541:ARG:HB3	2.21	0.55
2:B:2023:THR:OG1	2:B:2024:PRO:HD2	2.06	0.55
2:B:2302:LEU:HD22	2:B:2302:LEU:H	1.71	0.55
2:B:1709:TYR:HE2	2:B:1924:TYR:HA	1.71	0.55
2:B:2042:GLN:HE21	2:B:2047:ALA:CB	2.20	0.55
2:B:1864:ASN:HB3	2:B:1867:HIS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1976:TYR:CE2	2:B:1984:GLU:CD	2.80	0.55
2:B:2246:GLN:OE1	2:B:2320:ARG:HB2	2.06	0.55
1:A:164:LEU:O	1:A:167:ASP:O	2.25	0.55
1:A:673:PHE:O	1:A:674:SER:HB2	2.06	0.55
2:B:1733:VAL:O	2:B:1850:GLY:C	2.45	0.55
2:B:1796:GLN:O	2:B:1797:ARG:HB3	2.07	0.55
1:A:660:HIS:HB2	1:A:680:MET:HG3	1.89	0.55
1:A:237:TYR:CZ	1:A:242:LEU:HB2	2.42	0.54
1:A:457:VAL:HA	1:A:515:VAL:HG12	1.88	0.54
2:B:2027:MET:HE2	2:B:2032:ILE:HD13	1.89	0.54
2:B:2046:TRP:CZ3	2:B:2059:ILE:CB	2.89	0.54
1:A:536:PHE:CD1	1:A:536:PHE:N	2.75	0.54
1:A:664:TYR:HE1	2:B:1826:THR:N	2.05	0.54
2:B:1732:LYS:NZ	2:B:1918:PHE:HE2	2.04	0.54
1:A:3:ARG:HH22	1:A:79:GLU:CD	2.11	0.54
1:A:172:LEU:N	1:A:172:LEU:HD12	2.22	0.54
1:A:475:ILE:O	1:A:475:ILE:CG2	2.56	0.54
1:A:495:VAL:CG2	1:A:496:LYS:N	2.70	0.54
2:B:1735:PHE:CE1	2:B:1851:LEU:CB	2.90	0.54
2:B:1975:LEU:N	2:B:1975:LEU:HD23	2.22	0.54
1:A:393:TRP:HA	1:A:393:TRP:CE3	2.43	0.54
1:A:660:HIS:ND1	1:A:680:MET:CE	2.71	0.54
2:B:1705:ARG:NH2	2:B:1707:TRP:HZ3	2.05	0.54
2:B:2026:GLY:O	2:B:2032:ILE:HB	2.07	0.54
1:A:168:LEU:H	1:A:172:LEU:HB2	1.71	0.54
1:A:100:ALA:CB	1:A:138:TRP:CE3	2.90	0.54
1:A:269:ILE:HD12	1:A:288:ILE:HG21	1.89	0.54
1:A:503:ILE:HG21	1:A:537:VAL:HG13	1.88	0.54
1:A:640:LEU:HB3	1:A:677:THR:CB	2.38	0.54
2:B:2245:THR:C	2:B:2286:ASN:ND2	2.56	0.54
2:B:2273:LEU:HD22	2:B:2280:VAL:CG2	2.36	0.54
1:A:640:LEU:HB2	1:A:677:THR:HB	1.89	0.54
2:B:1833:LYS:HG3	2:B:1834:ALA:H	1.73	0.54
2:B:1840:ASP:O	2:B:1841:VAL:HB	2.07	0.54
3:C:3:BMA:C6	3:C:4:MAN:H5	2.38	0.54
1:A:111:GLY:O	1:A:161:HIS:HB3	2.07	0.54
1:A:688:TRP:HZ2	2:B:1799:GLY:HA2	1.73	0.54
2:B:1953:ILE:HD12	2:B:1953:ILE:N	2.23	0.54
2:B:2180:MET:CE	2:B:2232:VAL:HG11	2.38	0.54
1:A:398:LEU:HD23	1:A:399:VAL:H	1.73	0.54
1:A:662:MET:O	1:A:663:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1890:TYR:O	2:B:1894:ASN:N	2.22	0.54
2:B:2070:TRP:CE3	2:B:2150:ARG:HD2	2.43	0.54
2:B:2156:TYR:HB2	2:B:2159:ARG:O	2.08	0.54
1:A:425:LYS:NZ	1:A:581:GLU:OE1	2.41	0.53
1:A:492:PRO:O	1:A:494:GLY:N	2.33	0.53
2:B:1830:PHE:CZ	2:B:1987:GLU:HG3	2.44	0.53
2:B:1963:PHE:HB2	2:B:1986:VAL:HG11	1.89	0.53
1:A:426:VAL:HG22	1:A:586:TYR:HE1	1.73	0.53
2:B:2023:THR:HB	2:B:2176:MET:CE	2.38	0.53
2:B:2200:PHE:O	2:B:2202:THR:HG23	2.08	0.53
1:A:114:TYR:CE2	2:B:1997:ARG:CB	2.62	0.53
1:A:536:PHE:N	1:A:536:PHE:HD1	2.06	0.53
2:B:1830:PHE:HE2	2:B:1986:VAL:HA	1.74	0.53
2:B:2039:ALA:HB2	2:B:2048:PRO:CG	2.31	0.53
2:B:2064:THR:OG1	2:B:2065:LYS:N	2.39	0.53
2:B:2274:PHE:CD1	2:B:2275:PHE:N	2.76	0.53
1:A:148:ALA:CA	1:A:180:ARG:HH21	2.19	0.53
1:A:267:HIS:HA	1:A:312:ILE:HD11	1.90	0.53
1:A:426:VAL:HG22	1:A:586:TYR:CE1	2.43	0.53
1:A:428:PHE:CE2	1:A:475:ILE:CG1	2.90	0.53
1:A:65:ARG:HB3	1:A:66:PRO:HD3	1.87	0.53
1:A:242:LEU:HD12	1:A:243:PRO:N	2.24	0.53
1:A:465:PHE:CD1	1:A:466:LYS:N	2.77	0.53
2:B:1699:PHE:CD1	2:B:1740:ASP:OD1	2.61	0.53
2:B:1884:ASP:HA	2:B:1917:ARG:HG2	1.91	0.53
2:B:2013:LEU:N	2:B:2013:LEU:CD2	2.72	0.53
1:A:99:HIS:HD2	1:A:161:HIS:ND1	2.06	0.53
2:B:2190:ILE:HG12	2:B:2232:VAL:HG12	1.90	0.53
1:A:385:TYR:CE1	1:A:436:PHE:HB3	2.44	0.53
1:A:527:ARG:HD2	1:A:527:ARG:N	2.23	0.53
2:B:1830:PHE:HD2	2:B:1985:THR:OG1	1.90	0.53
2:B:1870:GLN:HG3	2:B:1871:VAL:H	1.74	0.53
2:B:1976:TYR:CE2	2:B:1984:GLU:OE1	2.62	0.53
1:A:688:TRP:NE1	2:B:1799:GLY:HA2	2.24	0.53
1:A:498:LEU:H	1:A:498:LEU:CD1	2.10	0.53
1:A:578:VAL:HG23	1:A:644:ALA:H	1.73	0.53
2:B:2196:PHE:HD1	2:B:2222:GLN:O	1.92	0.53
2:B:2275:PHE:HA	2:B:2280:VAL:HA	1.91	0.53
2:B:1973:MET:HE3	2:B:1976:TYR:CB	2.34	0.53
2:B:2027:MET:CA	2:B:2032:ILE:HD12	2.39	0.53
1:A:80:VAL:O	1:A:81:TYR:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LEU:HD12	1:A:671:PHE:N	2.16	0.52
2:B:1755:HIS:CE1	2:B:1756:LEU:CD2	2.92	0.52
2:B:2210:LEU:HG	2:B:2211:HIS:ND1	2.24	0.52
2:B:2244:THR:OG1	2:B:2322:GLU:HB3	2.09	0.52
1:A:99:HIS:ND1	1:A:100:ALA:N	2.56	0.52
1:A:308:LEU:HG	1:A:322:ALA:O	2.09	0.52
1:A:673:PHE:O	1:A:674:SER:CB	2.56	0.52
2:B:1946:SER:CA	2:B:1978:LEU:HD12	2.40	0.52
2:B:1995:ILE:N	2:B:1995:ILE:HD13	2.24	0.52
2:B:2081:ILE:HA	2:B:2168:GLY:CA	2.39	0.52
2:B:2304:ARG:HD2	2:B:2305:TYR:CZ	2.44	0.52
1:A:168:LEU:HA	1:A:172:LEU:HB2	1.91	0.52
1:A:249:HIS:O	1:A:300:LEU:O	2.26	0.52
1:A:393:TRP:HA	1:A:393:TRP:HE3	1.75	0.52
1:A:484:ARG:HH11	1:A:486:LEU:HA	1.74	0.52
2:B:2087:GLN:N	2:B:2163:ARG:O	2.42	0.52
1:A:308:LEU:HD12	1:A:308:LEU:C	2.30	0.52
2:B:1855:LEU:HD23	2:B:1856:LEU:N	2.25	0.52
2:B:2226:PRO:O	2:B:2310:PRO:O	2.26	0.52
2:B:2261:LEU:HD21	2:B:2281:LYS:O	2.09	0.52
2:B:2281:LYS:HD3	2:B:2282:VAL:N	2.25	0.52
1:A:14:TRP:N	1:A:46:TYR:O	2.43	0.52
1:A:527:ARG:O	1:A:528:CYS:HB2	2.09	0.52
1:A:576:PHE:HE2	1:A:650:SER:HB3	1.74	0.52
1:A:580:ASP:C	1:A:582:ASN:H	2.13	0.52
2:B:1732:LYS:HB3	2:B:1849:SER:O	2.10	0.52
2:B:1932:LEU:CB	2:B:2014:PHE:HA	2.40	0.52
2:B:2273:LEU:HD21	2:B:2280:VAL:HG23	1.73	0.52
1:A:278:VAL:HG12	1:A:296:ALA:CB	2.38	0.52
1:A:398:LEU:CG	1:A:399:VAL:H	2.22	0.52
2:B:1932:LEU:HB3	2:B:2014:PHE:HA	1.91	0.52
2:B:2261:LEU:CD2	2:B:2281:LYS:O	2.58	0.52
2:B:2262:ILE:HD11	2:B:2283:PHE:CD1	2.45	0.52
1:A:155:THR:HG21	1:A:256:HIS:HA	1.90	0.52
1:A:501:PHE:O	1:A:503:ILE:N	2.42	0.52
1:A:622:PHE:O	1:A:623:ASP:OD1	2.28	0.52
1:A:65:ARG:HB3	1:A:66:PRO:HD2	1.92	0.52
1:A:156:TYR:HA	1:A:293:PHE:CD2	2.45	0.52
1:A:396:ALA:CB	1:A:397:PRO:HA	2.24	0.52
2:B:1769:ASP:OD1	2:B:1769:ASP:N	2.32	0.52
2:B:2048:PRO:HG3	2:B:2062:TRP:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2264:SER:HB3	2:B:2301:LEU:HD22	1.91	0.52
1:A:438:THR:OG1	1:A:439:ARG:N	2.43	0.51
1:A:111:GLY:HA2	1:A:126:ASP:HA	1.91	0.51
1:A:654:SER:H	1:A:657:THR:HA	1.75	0.51
2:B:1829:GLU:CB	2:B:1966:ARG:HH11	2.22	0.51
2:B:1834:ALA:HB1	2:B:1945:LEU:HD11	1.91	0.51
1:A:51:PHE:CD2	1:A:158:TYR:HE1	2.28	0.51
2:B:2260:PHE:O	2:B:2283:PHE:HB2	2.11	0.51
1:A:14:TRP:CE2	1:A:71:LEU:CD1	2.93	0.51
1:A:237:TYR:CG	1:A:242:LEU:CB	2.90	0.51
1:A:656:TYR:CE1	2:B:1791:SER:CB	2.90	0.51
1:A:656:TYR:CD1	2:B:1791:SER:HB2	2.45	0.51
2:B:1704:GLU:HG2	2:B:1731:LYS:HE2	1.91	0.51
2:B:1766:GLU:CD	2:B:1860:THR:O	2.49	0.51
2:B:1975:LEU:HD23	2:B:1975:LEU:H	1.75	0.51
2:B:1733:VAL:H	2:B:1850:GLY:HA2	1.75	0.51
2:B:1840:ASP:O	2:B:1841:VAL:CG2	2.58	0.51
2:B:1983:PHE:CD1	2:B:1984:GLU:CA	2.93	0.51
2:B:2052:ARG:HH11	2:B:2165:GLU:HG3	1.76	0.51
2:B:2104:MET:HA	2:B:2113:GLN:O	2.11	0.51
1:A:80:VAL:HA	1:A:140:VAL:HG11	1.92	0.51
1:A:97:SER:O	1:A:160:SER:HA	2.11	0.51
1:A:274:HIS:HE2	1:A:306:PHE:HE2	1.59	0.51
1:A:496:LYS:O	1:A:500:ASP:HB2	2.09	0.51
1:A:528:CYS:HA	1:A:553:ILE:O	2.11	0.51
1:A:658:PHE:HZ	1:A:684:ASN:ND2	2.07	0.51
2:B:2129:ASN:CB	2:B:2134:GLY:HA3	2.41	0.51
1:A:162:VAL:HG23	1:A:167:ASP:OD2	2.11	0.51
1:A:272:GLU:CB	1:A:307:LEU:H	2.24	0.51
2:B:2171:LEU:HD12	2:B:2171:LEU:H	1.75	0.51
2:B:2322:GLU:HG3	2:B:2323:VAL:N	2.26	0.51
2:B:1889:TRP:CE3	2:B:1890:TYR:N	2.79	0.51
1:A:526:PRO:C	1:A:679:PHE:HZ	2.14	0.51
1:A:631:LEU:CD2	1:A:632:HIS:ND1	2.71	0.51
2:B:1952:ASN:HB3	2:B:1954:HIS:CD2	2.45	0.51
1:A:147:MET:CE	2:B:1972:LYS:NZ	2.74	0.51
1:A:199:PHE:CD1	1:A:269:ILE:HD13	2.46	0.51
1:A:625:LEU:O	1:A:627:LEU:N	2.39	0.51
1:A:461:LEU:HD22	1:A:513:TRP:CE3	2.46	0.50
1:A:581:GLU:O	1:A:584:SER:HB3	2.11	0.50
1:A:687:LEU:HA	1:A:710:SER:OG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1787:SER:H	2:B:1790:ILE:HG13	1.75	0.50
2:B:2063:SER:OG	2:B:2161:THR:HB	2.11	0.50
1:A:271:LEU:HA	1:A:308:LEU:HA	1.92	0.50
1:A:501:PHE:O	1:A:502:PRO:C	2.47	0.50
1:A:679:PHE:CD1	1:A:679:PHE:N	2.78	0.50
2:B:1707:TRP:HA	2:B:1707:TRP:HE3	1.72	0.50
2:B:1795:ASP:CG	2:B:1800:ALA:HB2	2.32	0.50
2:B:2186:SER:HB2	2:B:2189:GLN:HG3	1.93	0.50
2:B:2195:TYR:HA	2:B:2220:ARG:O	2.11	0.50
1:A:688:TRP:HZ2	2:B:1799:GLY:CA	2.23	0.50
2:B:2062:TRP:CZ3	2:B:2071:ILE:HB	2.47	0.50
1:A:87:THR:HG22	1:A:135:THR:OG1	2.11	0.50
1:A:94:HIS:HD2	1:A:95:PRO:HD2	1.77	0.50
1:A:137:VAL:HG11	2:B:2329:GLN:HE22	1.76	0.50
1:A:417:GLN:NE2	1:A:602:GLN:HB2	2.26	0.50
1:A:509:PHE:HD1	1:A:510:LYS:N	2.08	0.50
1:A:631:LEU:HD23	1:A:631:LEU:C	2.31	0.50
2:B:2331:LEU:HD23	2:B:2331:LEU:N	2.26	0.50
1:A:2:THR:HB	1:A:82:ASP:OD2	2.11	0.50
1:A:105:TYR:HD2	1:A:110:GLU:HB3	1.71	0.50
1:A:106:TRP:CZ3	2:B:2329:GLN:HB3	2.46	0.50
1:A:206:LYS:O	1:A:207:SER:HB3	2.12	0.50
2:B:1808:LYS:O	2:B:1811:GLU:HB2	2.12	0.50
2:B:1983:PHE:O	2:B:1984:GLU:CB	2.52	0.50
1:A:270:PHE:O	1:A:308:LEU:HA	2.11	0.50
1:A:617:ILE:CG1	1:A:706:LEU:HD22	2.40	0.50
1:A:654:SER:HB2	1:A:690:LEU:HD12	1.93	0.50
1:A:688:TRP:CZ2	2:B:1799:GLY:CA	2.94	0.50
2:B:2052:ARG:HD3	2:B:2165:GLU:CG	2.42	0.50
2:B:2265:SER:OG	2:B:2271:TRP:CE3	2.61	0.50
1:A:616:SER:OG	1:A:617:ILE:N	2.45	0.50
2:B:1752:LEU:HD12	2:B:1752:LEU:N	2.27	0.50
1:A:121:ARG:HG3	1:A:121:ARG:NH1	2.24	0.50
2:B:1830:PHE:CE1	2:B:1966:ARG:CZ	2.95	0.50
2:B:1877:ALA:HA	2:B:1943:TYR:HB2	1.93	0.50
2:B:1947:MET:HE3	2:B:1948:GLY:N	2.24	0.50
2:B:2042:GLN:HB3	2:B:2062:TRP:NE1	2.26	0.50
2:B:2046:TRP:CD1	2:B:2159:ARG:NH2	2.79	0.50
1:A:578:VAL:CG2	1:A:644:ALA:H	2.25	0.50
2:B:1908:GLU:O	2:B:1909:ASP:OD1	2.30	0.50
2:B:1941:ARG:HD2	2:B:1943:TYR:OH	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:NAG:O3	3:C:3:BMA:O6	2.30	0.50
1:A:5:TYR:CD2	1:A:76:ILE:HB	2.36	0.49
1:A:158:TYR:CZ	1:A:174:GLY:HA3	2.47	0.49
1:A:527:ARG:O	1:A:679:PHE:CE2	2.65	0.49
1:A:647:ASP:CG	2:B:1950:ASN:HD21	2.15	0.49
1:A:232:HIS:CD2	1:A:318:ASP:CB	2.95	0.49
1:A:299:LEU:H	1:A:299:LEU:HD23	1.77	0.49
1:A:316:GLN:CD	1:A:316:GLN:H	2.15	0.49
1:A:480:ILE:CG2	1:A:481:THR:N	2.70	0.49
1:A:624:SER:O	1:A:625:LEU:HD12	2.12	0.49
1:A:653:PHE:HB2	1:A:693:HIS:CE1	2.42	0.49
1:A:687:LEU:CD1	1:A:688:TRP:H	2.25	0.49
2:B:2220:ARG:HH11	2:B:2220:ARG:CG	2.25	0.49
1:A:626:GLN:HA	1:A:707:LYS:HB2	1.93	0.49
1:A:656:TYR:HB2	1:A:686:GLY:C	2.32	0.49
1:A:107:LYS:O	1:A:126:ASP:OD1	2.30	0.49
1:A:392:ASP:HA	1:A:424:LYS:HA	1.94	0.49
2:B:2083:GLY:HA2	2:B:2140:PHE:CE2	2.44	0.49
2:B:2195:TYR:HD2	2:B:2204:SER:HA	1.76	0.49
1:A:57:HIS:O	1:A:58:LEU:CG	2.61	0.49
1:A:267:HIS:HB2	1:A:288:ILE:HG23	1.95	0.49
1:A:386:ILE:O	1:A:465:PHE:HA	2.13	0.49
1:A:626:GLN:C	1:A:627:LEU:HD12	2.32	0.49
2:B:1807:VAL:HG13	2:B:1811:GLU:HB3	1.94	0.49
1:A:100:ALA:HB3	1:A:105:TYR:CE1	2.48	0.49
2:B:1828:ASP:OD2	2:B:1968:LYS:C	2.51	0.49
2:B:2210:LEU:HD13	2:B:2321:MET:HA	1.94	0.49
1:A:10:VAL:HB	1:A:52:VAL:HG11	1.95	0.49
1:A:319:GLY:O	1:A:320:MET:HB2	2.12	0.49
2:B:1735:PHE:CE1	2:B:1851:LEU:HG	2.40	0.49
2:B:2230:LEU:O	2:B:2308:ILE:HG22	2.11	0.49
1:A:137:VAL:HG11	2:B:2329:GLN:NE2	2.27	0.49
1:A:249:HIS:CE1	1:A:303:LEU:CD1	2.96	0.49
1:A:423:TYR:CD2	1:A:581:GLU:HG3	2.47	0.49
1:A:700:ARG:HH11	2:B:1843:LEU:HB3	1.77	0.49
2:B:2105:TYR:HB2	2:B:2146:ALA:CB	2.43	0.49
2:B:2144:ILE:HG22	2:B:2145:ILE:N	2.27	0.49
2:B:2275:PHE:CD1	2:B:2275:PHE:N	2.81	0.49
1:A:101:VAL:O	1:A:101:VAL:HG13	2.13	0.49
1:A:663:VAL:HG13	2:B:1968:LYS:HD2	1.95	0.49
1:A:688:TRP:HE1	2:B:1799:GLY:CA	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HB3	1:A:130:PRO:HD3	1.94	0.49
1:A:660:HIS:HB3	1:A:682:MET:HG3	1.95	0.49
1:A:688:TRP:CD1	2:B:1800:ALA:HB3	2.48	0.49
2:B:1838:PHE:CE1	2:B:1852:ILE:HG13	2.48	0.49
2:B:1946:SER:CB	2:B:1978:LEU:CB	2.86	0.48
2:B:1968:LYS:O	2:B:1969:GLU:HG2	2.13	0.48
2:B:2325:GLY:C	2:B:2326:CYS:SG	2.91	0.48
1:A:472:PRO:HB2	1:A:503:ILE:HB	1.96	0.48
1:A:655:GLY:HA3	1:A:687:LEU:HB3	1.95	0.48
2:B:1755:HIS:ND1	2:B:1756:LEU:HD23	2.28	0.48
2:B:1779:ALA:O	2:B:1809:PRO:HG3	2.13	0.48
2:B:1924:TYR:HD1	2:B:1928:THR:HB	1.78	0.48
2:B:1996:TRP:HB2	2:B:2014:PHE:CE1	2.48	0.48
2:B:2330:ASP:C	2:B:2331:LEU:HD23	2.33	0.48
1:A:186:LYS:O	1:A:189:THR:N	2.46	0.48
1:A:200:ALA:CB	1:A:202:PHE:CE1	2.96	0.48
1:A:433:ASP:OD1	1:A:433:ASP:N	2.46	0.48
1:A:249:HIS:NE2	1:A:303:LEU:CD1	2.71	0.48
1:A:282:ARG:HH12	1:A:299:LEU:CD2	2.26	0.48
1:A:473:TYR:HA	1:A:537:VAL:HG21	1.95	0.48
2:B:1873:VAL:HG21	2:B:1941:ARG:NH2	2.29	0.48
2:B:1944:LEU:HD23	2:B:1944:LEU:N	2.28	0.48
2:B:2027:MET:HE3	2:B:2032:ILE:HD13	1.93	0.48
1:A:653:PHE:HB3	1:A:691:GLY:O	2.13	0.48
2:B:2106:SER:O	2:B:2146:ALA:HB1	2.13	0.48
1:A:13:SER:HB3	1:A:47:LYS:HG2	1.95	0.48
1:A:249:HIS:CE1	1:A:303:LEU:HD12	2.48	0.48
1:A:542:ASP:O	1:A:543:LEU:C	2.52	0.48
1:A:621:VAL:CG1	1:A:622:PHE:H	1.90	0.48
1:A:657:THR:CG2	2:B:1788:SER:HA	2.18	0.48
2:B:1732:LYS:NZ	2:B:1918:PHE:CE2	2.80	0.48
2:B:2087:GLN:HG2	2:B:2163:ARG:HB2	1.94	0.48
2:B:2246:GLN:OE1	2:B:2320:ARG:NE	2.46	0.48
2:B:2331:LEU:O	2:B:2332:TYR:CB	2.62	0.48
1:A:237:TYR:HD2	1:A:241:SER:HB2	1.79	0.48
1:A:473:TYR:O	1:A:504:LEU:HD12	2.12	0.48
1:A:664:TYR:CD1	2:B:1826:THR:CG2	2.95	0.48
1:A:471:ARG:CB	1:A:585:TRP:CE3	2.97	0.48
1:A:518:GLU:H	1:A:518:GLU:CD	2.18	0.48
1:A:586:TYR:O	1:A:590:ASN:ND2	2.47	0.48
2:B:1735:PHE:HE1	2:B:1851:LEU:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2101:PHE:HD2	2:B:2151:LEU:HG	1.78	0.48
2:B:2025:LEU:HD12	2:B:2166:LEU:HD12	1.96	0.48
1:A:51:PHE:CE1	1:A:172:LEU:HA	2.49	0.47
1:A:237:TYR:CD2	1:A:242:LEU:CB	2.96	0.47
1:A:659:LYS:HE2	2:B:1822:HIS:CD2	2.49	0.47
1:A:670:LEU:CD1	1:A:671:PHE:H	2.19	0.47
1:A:84:VAL:HG23	1:A:138:TRP:CD1	2.49	0.47
1:A:653:PHE:O	1:A:690:LEU:HA	2.14	0.47
2:B:1766:GLU:HB3	2:B:1769:ASP:OD1	2.14	0.47
2:B:2238:MET:CE	2:B:2326:CYS:O	2.62	0.47
1:A:311:HIS:O	1:A:312:ILE:CG1	2.59	0.47
1:A:398:LEU:HG	1:A:399:VAL:H	1.79	0.47
1:A:542:ASP:O	1:A:545:SER:HB2	2.15	0.47
1:A:676:GLU:OE1	1:A:676:GLU:HA	2.14	0.47
2:B:1709:TYR:CD1	2:B:1709:TYR:N	2.81	0.47
2:B:1732:LYS:CB	2:B:1849:SER:O	2.62	0.47
2:B:1936:GLN:HG2	2:B:1937:ASP:OD1	2.15	0.47
2:B:2087:GLN:HB3	2:B:2163:ARG:CA	2.44	0.47
1:A:163:ASP:HA	2:B:2007:HIS:NE2	2.29	0.47
2:B:2329:GLN:CG	2:B:2332:TYR:O	2.37	0.47
1:A:664:TYR:OH	2:B:1825:PRO:CA	2.62	0.47
1:A:712:ASP:O	1:A:713:LYS:HG2	2.14	0.47
2:B:1830:PHE:HE1	2:B:1966:ARG:NH2	2.12	0.47
2:B:1888:SER:OG	2:B:1889:TRP:N	2.46	0.47
2:B:2178:LEU:O	2:B:2185:ILE:HD12	2.14	0.47
1:A:380:LYS:CG	1:A:382:TRP:HZ3	2.27	0.47
1:A:471:ARG:N	1:A:471:ARG:HD3	2.30	0.47
1:A:654:SER:CB	1:A:690:LEU:HB2	2.45	0.47
1:A:661:LYS:HA	1:A:665:GLU:HA	1.97	0.47
2:B:1963:PHE:CB	2:B:1986:VAL:HG11	2.45	0.47
2:B:2027:MET:CB	2:B:2165:GLU:HG2	2.42	0.47
2:B:2052:ARG:HA	2:B:2163:ARG:HB3	1.95	0.47
2:B:2265:SER:O	2:B:2303:THR:HB	2.14	0.47
1:A:116:ASP:O	2:B:1995:ILE:HG13	2.15	0.47
1:A:432:THR:OG1	1:A:440:GLU:CG	2.62	0.47
1:A:663:VAL:CG1	2:B:1968:LYS:HD2	2.45	0.47
1:A:663:VAL:HG11	2:B:1968:LYS:HB2	1.95	0.47
1:A:693:HIS:HD2	1:A:695:SER:HB2	1.77	0.47
2:B:1739:THR:H	2:B:1746:PRO:CG	2.24	0.47
2:B:1969:GLU:HA	2:B:1969:GLU:OE1	2.15	0.47
2:B:1996:TRP:O	2:B:2013:LEU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2046:TRP:O	2:B:2062:TRP:HA	2.15	0.47
2:B:2054:HIS:O	2:B:2060:ASN:HB2	2.13	0.47
2:B:2105:TYR:HB2	2:B:2146:ALA:HB3	1.97	0.47
2:B:2231:GLN:HA	2:B:2306:LEU:O	2.14	0.47
1:A:127:LYS:CG	1:A:162:VAL:HG11	2.42	0.47
1:A:645:GLN:O	1:A:646:THR:HB	2.15	0.47
2:B:1785:PHE:HB3	2:B:1815:TYR:HE2	1.79	0.47
1:A:65:ARG:O	1:A:66:PRO:C	2.53	0.47
1:A:455:GLY:O	1:A:554:CYS:N	2.47	0.47
1:A:617:ILE:CG1	1:A:706:LEU:HD13	2.44	0.47
2:B:1889:TRP:CE3	2:B:1890:TYR:HB2	2.48	0.47
2:B:2083:GLY:N	2:B:2140:PHE:HD2	2.13	0.47
2:B:2156:TYR:HD2	2:B:2159:ARG:C	2.18	0.47
1:A:89:LYS:HA	1:A:133:SER:HA	1.97	0.46
1:A:278:VAL:CG2	1:A:279:ARG:H	2.24	0.46
1:A:663:VAL:HG13	2:B:1968:LYS:CB	2.41	0.46
2:B:1789:LEU:HD23	2:B:1823:MET:SD	2.54	0.46
1:A:398:LEU:CD2	1:A:399:VAL:H	2.28	0.46
1:A:576:PHE:HE2	1:A:650:SER:CB	2.28	0.46
1:A:607:GLU:O	1:A:611:SER:OG	2.32	0.46
2:B:2265:SER:OG	2:B:2270:GLN:O	2.33	0.46
2:B:1975:LEU:HD23	2:B:1975:LEU:O	2.15	0.46
1:A:182:GLY:O	1:A:186:LYS:CE	2.59	0.46
1:A:396:ALA:CB	1:A:397:PRO:CA	2.90	0.46
1:A:578:VAL:H	1:A:643:GLY:HA3	1.81	0.46
1:A:684:ASN:C	1:A:686:GLY:H	2.13	0.46
2:B:2265:SER:OG	2:B:2271:TRP:HA	2.16	0.46
2:B:2273:LEU:O	2:B:2275:PHE:HD1	1.93	0.46
3:C:1:NAG:O3	3:C:2:NAG:H62	2.15	0.46
1:A:486:LEU:CD2	1:A:487:TYR:CD2	2.98	0.46
1:A:534:SER:OG	1:A:535:SER:N	2.49	0.46
1:A:652:PHE:HD1	1:A:690:LEU:HD11	1.80	0.46
1:A:697:PHE:CD1	1:A:698:ARG:HB2	2.51	0.46
2:B:1771:ILE:HB	2:B:1817:TRP:NE1	2.31	0.46
2:B:2080:ILE:O	2:B:2080:ILE:HG13	2.15	0.46
1:A:181:GLU:HG3	1:A:182:GLY:N	2.30	0.46
2:B:1711:MET:SD	2:B:1711:MET:N	2.89	0.46
2:B:1882:ILE:HD11	2:B:1919:HIS:CE1	2.50	0.46
2:B:1947:MET:O	2:B:1952:ASN:ND2	2.48	0.46
2:B:2101:PHE:CE2	2:B:2103:ILE:HD11	2.50	0.46
2:B:2132:SER:O	2:B:2133:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2179:GLY:HA2	2:B:2184:ALA:HB3	1.98	0.46
2:B:1751:GLU:OE1	2:B:2105:TYR:OH	2.34	0.46
1:A:667:THR:C	1:A:669:THR:N	2.68	0.46
2:B:1758:LEU:HD12	2:B:1922:ASN:O	2.14	0.46
1:A:13:SER:HA	1:A:47:LYS:HA	1.97	0.46
1:A:303:LEU:HA	1:A:326:VAL:HG13	1.97	0.46
1:A:305:GLN:HG2	1:A:325:LYS:HG2	1.98	0.46
1:A:486:LEU:HD22	1:A:487:TYR:CD2	2.51	0.46
2:B:1705:ARG:HG2	2:B:1706:LEU:N	2.29	0.46
2:B:1797:ARG:O	2:B:1797:ARG:HD3	2.16	0.46
2:B:1821:HIS:O	2:B:1824:ALA:HB3	2.16	0.46
2:B:1886:THR:HG23	2:B:1887:LYS:HD2	1.98	0.46
1:A:80:VAL:HA	1:A:140:VAL:HG12	1.98	0.46
1:A:147:MET:HE1	2:B:1972:LYS:HZ2	1.81	0.46
1:A:398:LEU:HD23	1:A:399:VAL:N	2.31	0.46
2:B:2097:TYR:CE1	2:B:2130:VAL:HA	2.51	0.46
2:B:2105:TYR:HD2	2:B:2146:ALA:HB2	1.80	0.46
2:B:2212:LEU:O	2:B:2217:ASN:HB2	2.16	0.46
1:A:278:VAL:CG2	1:A:279:ARG:N	2.79	0.45
1:A:421:ARG:HG2	1:A:422:LYS:N	2.31	0.45
1:A:684:ASN:N	1:A:685:PRO:CD	2.79	0.45
2:B:2156:TYR:CD1	2:B:2156:TYR:N	2.83	0.45
2:B:2262:ILE:HG22	2:B:2306:LEU:HD21	1.97	0.45
1:A:198:LEU:H	1:A:235:ASN:HD22	1.63	0.45
1:A:200:ALA:HB3	1:A:202:PHE:CE1	2.51	0.45
1:A:426:VAL:HG11	1:A:473:TYR:HE2	1.80	0.45
1:A:473:TYR:O	1:A:504:LEU:HD11	2.16	0.45
1:A:688:TRP:HE1	2:B:1799:GLY:HA2	1.81	0.45
2:B:1771:ILE:O	2:B:1816:PHE:HA	2.16	0.45
2:B:2033:ARG:H	2:B:2036:GLN:NE2	2.14	0.45
1:A:137:VAL:O	1:A:137:VAL:HG13	2.16	0.45
1:A:184:LEU:HD23	1:A:184:LEU:O	2.16	0.45
1:A:187:GLU:HA	1:A:190:GLN:CB	2.33	0.45
1:A:288:ILE:HG23	1:A:288:ILE:O	2.16	0.45
1:A:595:LEU:HD11	1:A:601:VAL:HG21	1.98	0.45
2:B:1755:HIS:CE1	2:B:1756:LEU:HD23	2.51	0.45
2:B:1935:ALA:HB2	2:B:2017:TYR:CZ	2.52	0.45
2:B:2263:SER:HB2	2:B:2307:ARG:CB	2.46	0.45
1:A:576:PHE:N	1:A:640:LEU:O	2.49	0.45
1:A:668:LEU:HG	2:B:1788:SER:HG	1.81	0.45
2:B:1737:GLU:HG2	2:B:1761:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2286:ASN:H	2:B:2293:VAL:HG11	1.82	0.45
1:A:463:ILE:N	1:A:463:ILE:HD12	2.31	0.45
1:A:501:PHE:O	1:A:503:ILE:CG1	2.52	0.45
2:B:1889:TRP:HB3	2:B:1893:GLU:HG3	1.98	0.45
2:B:1963:PHE:CD1	2:B:1986:VAL:CG1	2.84	0.45
1:A:237:TYR:CD1	1:A:242:LEU:CB	3.00	0.45
1:A:577:SER:O	1:A:616:SER:OG	2.35	0.45
2:B:1708:ASP:C	2:B:1709:TYR:CD1	2.90	0.45
2:B:1755:HIS:CE1	2:B:1756:LEU:HD21	2.52	0.45
2:B:1834:ALA:HB3	2:B:1983:PHE:CD1	2.51	0.45
2:B:2080:ILE:HD12	2:B:2082:HIS:NE2	2.31	0.45
1:A:419:ILE:HG22	1:A:594:PHE:HB2	1.98	0.45
2:B:1975:LEU:N	2:B:1975:LEU:CD2	2.79	0.45
2:B:2028:ALA:HB2	2:B:2052:ARG:HH11	1.82	0.45
1:A:163:ASP:HA	2:B:2007:HIS:CE1	2.52	0.45
1:A:184:LEU:O	1:A:187:GLU:N	2.48	0.45
1:A:453:LEU:CD2	1:A:533:TYR:HE2	2.15	0.45
1:A:548:ILE:HG13	1:A:549:GLY:N	2.32	0.45
1:A:604:GLU:HA	1:A:608:PHE:CZ	2.52	0.45
1:A:651:VAL:CG1	1:A:652:PHE:N	2.80	0.45
1:A:688:TRP:HZ2	2:B:1799:GLY:H	1.63	0.45
2:B:1735:PHE:CE1	2:B:1851:LEU:CD2	3.00	0.45
2:B:2046:TRP:CH2	2:B:2058:SER:C	2.88	0.45
2:B:2048:PRO:O	2:B:2049:LYS:CB	2.65	0.45
2:B:2244:THR:HG22	2:B:2294:VAL:HB	1.99	0.45
2:B:2273:LEU:HD22	2:B:2280:VAL:CB	2.47	0.45
1:A:184:LEU:O	1:A:185:ALA:C	2.53	0.45
1:A:267:HIS:CE1	1:A:320:MET:HG3	2.52	0.45
1:A:499:LYS:O	1:A:536:PHE:O	2.35	0.45
1:A:610:ALA:HA	1:A:613:ILE:HG12	1.99	0.45
2:B:1789:LEU:O	2:B:1791:SER:N	2.50	0.45
2:B:1868:GLY:O	2:B:1869:ARG:HG3	2.16	0.45
2:B:2157:SER:C	2:B:2159:ARG:H	2.19	0.45
2:B:2234:PHE:HD2	2:B:2238:MET:HG3	1.82	0.45
2:B:2302:LEU:H	2:B:2302:LEU:CD2	2.30	0.45
1:A:381:THR:HB	1:A:460:THR:HB	1.99	0.45
1:A:530:THR:HB	1:A:677:THR:OG1	2.17	0.45
1:A:125:ASP:C	1:A:127:LYS:H	2.21	0.44
1:A:389:GLU:CD	1:A:431:TYR:CE2	2.90	0.44
1:A:617:ILE:HG12	1:A:706:LEU:CD1	2.47	0.44
1:A:663:VAL:HG12	1:A:664:TYR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1789:LEU:HD21	2:B:1835:TRP:NE1	2.32	0.44
2:B:1919:HIS:N	2:B:1919:HIS:CD2	2.85	0.44
2:B:2102:ILE:HD12	2:B:2152:HIS:HB2	1.98	0.44
3:C:3:BMA:H62	3:C:4:MAN:H5	1.99	0.44
1:A:503:ILE:C	1:A:504:LEU:HG	2.37	0.44
1:A:651:VAL:HG11	1:A:668:LEU:HA	1.97	0.44
2:B:1755:HIS:CD2	2:B:1876:PHE:CD1	3.04	0.44
2:B:1860:THR:O	2:B:1862:THR:OG1	2.36	0.44
2:B:1932:LEU:HB2	2:B:2015:LEU:HD12	1.97	0.44
2:B:2038:THR:HG23	2:B:2072:LYS:HB3	1.99	0.44
2:B:2200:PHE:CZ	2:B:2215:ARG:HD3	2.52	0.44
2:B:2260:PHE:CZ	2:B:2295:ASN:ND2	2.86	0.44
2:B:2081:ILE:CG1	2:B:2144:ILE:HB	2.42	0.44
2:B:2096:LEU:CD1	2:B:2159:ARG:HB3	2.44	0.44
1:A:68:TRP:CZ2	1:A:69:MET:HE2	2.53	0.44
1:A:491:LEU:CB	1:A:492:PRO:HD2	2.39	0.44
1:A:625:LEU:HD13	1:A:706:LEU:HD21	1.99	0.44
1:A:705:LEU:HD22	1:A:705:LEU:H	1.80	0.44
2:B:1934:MET:HB3	2:B:2016:VAL:CA	2.47	0.44
1:A:243:PRO:HB2	1:A:244:GLY:H	1.61	0.44
2:B:1851:LEU:C	2:B:1851:LEU:HD22	2.38	0.44
2:B:2275:PHE:N	2:B:2275:PHE:HD1	2.16	0.44
1:A:159:LEU:CD1	1:A:168:LEU:HD21	2.48	0.44
1:A:621:VAL:HG12	1:A:622:PHE:CD2	2.53	0.44
2:B:1929:LEU:HD22	2:B:2012:THR:HG21	2.00	0.44
2:B:2264:SER:CB	2:B:2301:LEU:HD23	2.45	0.44
1:A:263:THR:O	1:A:265:GLU:N	2.49	0.44
1:A:385:TYR:CG	1:A:436:PHE:O	2.70	0.44
1:A:683:GLU:CD	1:A:683:GLU:H	2.20	0.44
2:B:1865:PRO:C	2:B:1867:HIS:N	2.67	0.44
2:B:1878:LEU:HD11	2:B:1942:TRP:CZ3	2.52	0.44
2:B:1924:TYR:CD1	2:B:1928:THR:HB	2.53	0.44
2:B:1995:ILE:HD13	2:B:1995:ILE:H	1.83	0.44
2:B:2031:HIS:HB2	2:B:2294:VAL:CG1	2.47	0.44
2:B:1849:SER:HA	2:B:1888:SER:HB2	2.00	0.44
2:B:1934:MET:HE3	2:B:1940:ILE:CG2	2.45	0.44
5:E:6:MAN:O5	5:E:7:MAN:H2	2.17	0.44
1:A:663:VAL:CB	2:B:1968:LYS:HD2	2.46	0.44
2:B:1889:TRP:CD2	2:B:1890:TYR:N	2.82	0.44
2:B:2022:GLN:OE1	2:B:2082:HIS:HB2	2.17	0.44
1:A:477:PRO:HG3	1:A:513:TRP:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:PHE:HD1	1:A:648:PHE:HA	1.53	0.43
2:B:1973:MET:HE1	2:B:1976:TYR:CD1	2.53	0.43
1:A:4:ARG:HG2	1:A:5:TYR:N	2.32	0.43
1:A:94:HIS:CE1	1:A:207:SER:OG	2.71	0.43
1:A:476:TYR:CG	1:A:477:PRO:HD2	2.53	0.43
1:A:656:TYR:HD2	1:A:659:LYS:NZ	2.16	0.43
1:A:683:GLU:C	1:A:685:PRO:HD2	2.39	0.43
2:B:2273:LEU:O	2:B:2275:PHE:HE1	1.96	0.43
1:A:4:ARG:HG3	1:A:85:VAL:O	2.18	0.43
1:A:234:VAL:O	1:A:235:ASN:HB2	2.18	0.43
1:A:412:LEU:CA	1:A:420:GLY:HA3	2.42	0.43
1:A:421:ARG:HG2	1:A:422:LYS:H	1.83	0.43
1:A:461:LEU:HB3	1:A:463:ILE:CD1	2.49	0.43
1:A:496:LYS:HD3	1:A:496:LYS:HA	1.69	0.43
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.54	0.43
2:B:1763:ILE:O	2:B:1763:ILE:CG2	2.66	0.43
2:B:2052:ARG:CD	2:B:2165:GLU:CB	2.72	0.43
2:B:2229:TRP:HA	2:B:2308:ILE:O	2.18	0.43
1:A:291:ILE:HG23	2:B:1955:SER:OG	2.18	0.43
1:A:509:PHE:CD1	1:A:510:LYS:N	2.86	0.43
1:A:627:LEU:HD13	1:A:707:LYS:O	2.18	0.43
2:B:1958:PHE:O	2:B:1959:SER:C	2.56	0.43
1:A:137:VAL:HG11	2:B:2329:GLN:OE1	2.19	0.43
1:A:412:LEU:C	1:A:420:GLY:HA3	2.39	0.43
1:A:432:THR:CB	1:A:433:ASP:OD1	2.65	0.43
1:A:526:PRO:O	1:A:679:PHE:CZ	2.59	0.43
1:A:652:PHE:C	1:A:657:THR:O	2.56	0.43
2:B:1756:LEU:N	2:B:1756:LEU:CD2	2.81	0.43
2:B:1922:ASN:HD22	2:B:1929:LEU:HD11	1.82	0.43
2:B:2075:LEU:C	2:B:2076:LEU:HG	2.38	0.43
2:B:1787:SER:H	2:B:1790:ILE:CG1	2.31	0.43
2:B:1922:ASN:HB2	2:B:1929:LEU:HD11	2.01	0.43
2:B:1934:MET:CB	2:B:2016:VAL:HA	2.48	0.43
2:B:2252:LEU:HD13	2:B:2252:LEU:O	2.18	0.43
2:B:2314:VAL:O	2:B:2315:HIS:HB2	2.19	0.43
1:A:86:ILE:HD12	1:A:98:LEU:HD21	2.01	0.43
1:A:309:PHE:HA	1:A:321:GLU:HA	2.01	0.43
1:A:580:ASP:O	1:A:582:ASN:N	2.44	0.43
2:B:1933:VAL:HG23	2:B:1933:VAL:O	2.19	0.43
1:A:198:LEU:H	1:A:235:ASN:ND2	2.17	0.43
1:A:385:TYR:CD1	1:A:436:PHE:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TYR:CE2	1:A:436:PHE:O	2.71	0.43
1:A:393:TRP:HD1	1:A:395:TYR:HE1	1.63	0.43
2:B:2106:SER:OG	2:B:2107:LEU:N	2.51	0.43
1:A:83:THR:HG22	1:A:140:VAL:N	2.24	0.43
1:A:267:HIS:HE1	1:A:320:MET:HG3	1.84	0.43
1:A:467:ASN:HB3	1:A:504:LEU:O	2.19	0.43
1:A:651:VAL:O	1:A:693:HIS:ND1	2.49	0.43
2:B:1782:PRO:HG3	2:B:1808:LYS:HA	2.00	0.43
1:A:427:ARG:CD	1:A:448:ILE:HA	2.49	0.42
2:B:2052:ARG:HD3	2:B:2165:GLU:HG3	2.01	0.42
3:C:2:NAG:O3	3:C:3:BMA:H4	2.19	0.42
1:A:391:GLU:HG2	1:A:392:ASP:N	2.35	0.42
1:A:396:ALA:CB	1:A:421:ARG:HH12	2.32	0.42
1:A:688:TRP:HZ2	2:B:1799:GLY:N	2.16	0.42
2:B:2286:ASN:H	2:B:2293:VAL:CG1	2.32	0.42
1:A:90:ASN:HD21	1:A:95:PRO:HA	1.84	0.42
2:B:1966:ARG:HA	2:B:1969:GLU:O	2.19	0.42
2:B:2076:LEU:C	2:B:2147:ARG:HE	2.22	0.42
1:A:86:ILE:HG22	1:A:87:THR:N	2.35	0.42
1:A:169:ASN:O	1:A:170:SER:CB	2.65	0.42
1:A:202:PHE:O	1:A:231:MET:HB2	2.19	0.42
1:A:602:GLN:OE1	1:A:602:GLN:HA	2.20	0.42
1:A:620:TYR:O	1:A:621:VAL:CB	2.67	0.42
2:B:1785:PHE:HB3	2:B:1815:TYR:CE2	2.55	0.42
2:B:1929:LEU:HA	2:B:1930:PRO:HD3	1.73	0.42
2:B:1973:MET:CE	2:B:1976:TYR:CD1	3.02	0.42
2:B:2039:ALA:C	2:B:2041:GLY:H	2.22	0.42
1:A:168:LEU:N	1:A:172:LEU:HD13	2.34	0.42
1:A:307:LEU:HD12	1:A:322:ALA:C	2.40	0.42
1:A:537:VAL:HB	1:A:542:ASP:OD1	2.20	0.42
1:A:542:ASP:O	1:A:545:SER:CB	2.68	0.42
2:B:1889:TRP:NE1	2:B:1892:THR:CG2	2.83	0.42
2:B:2045:GLN:O	2:B:2047:ALA:N	2.47	0.42
2:B:2193:SER:HA	2:B:2229:TRP:CE2	2.54	0.42
1:A:87:THR:HA	1:A:135:THR:HA	2.00	0.42
1:A:94:HIS:CD2	1:A:95:PRO:HD2	2.55	0.42
1:A:98:LEU:HB3	1:A:136:TYR:CE1	2.55	0.42
1:A:417:GLN:CD	1:A:601:VAL:HG22	2.29	0.42
1:A:504:LEU:HD23	1:A:509:PHE:HB2	2.01	0.42
2:B:2000:CYS:HB3	2:B:2010:MET:HG2	2.01	0.42
2:B:2042:GLN:HB2	2:B:2063:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2181:GLU:C	2:B:2183:LYS:H	2.23	0.42
1:A:270:PHE:HB2	1:A:309:PHE:CE1	2.47	0.42
1:A:393:TRP:NE1	1:A:448:ILE:HG23	2.35	0.42
1:A:432:THR:HG22	1:A:433:ASP:OD1	2.19	0.42
1:A:504:LEU:CD2	1:A:509:PHE:HB2	2.50	0.42
1:A:509:PHE:HB3	1:A:511:TYR:CE1	2.53	0.42
2:B:2156:TYR:N	2:B:2156:TYR:HD1	2.17	0.42
2:B:2180:MET:HE3	2:B:2232:VAL:HG11	2.01	0.42
2:B:2211:HIS:CE1	2:B:2292:PRO:HG3	2.55	0.42
1:A:14:TRP:CE2	1:A:71:LEU:HD13	2.54	0.42
1:A:232:HIS:CD2	1:A:318:ASP:HB3	2.55	0.42
1:A:640:LEU:HB3	1:A:677:THR:OG1	2.20	0.42
1:A:645:GLN:CD	1:A:645:GLN:N	2.73	0.42
2:B:1924:TYR:HB3	2:B:1928:THR:HB	2.02	0.42
2:B:1951:GLU:O	2:B:1953:ILE:CD1	2.68	0.42
1:A:428:PHE:HE2	1:A:475:ILE:HG13	1.82	0.42
1:A:687:LEU:HA	1:A:687:LEU:HD22	1.89	0.42
2:B:1863:LEU:HB2	2:B:1870:GLN:N	2.27	0.42
2:B:2311:GLN:O	2:B:2313:TRP:CD1	2.73	0.42
2:B:2329:GLN:C	2:B:2332:TYR:O	2.55	0.42
1:A:453:LEU:CD2	1:A:533:TYR:CD2	3.00	0.42
1:A:685:PRO:HG2	2:B:1822:HIS:CE1	2.52	0.42
1:A:687:LEU:HD13	1:A:688:TRP:H	1.85	0.42
1:A:155:THR:HG23	1:A:295:THR:OG1	2.20	0.41
1:A:605:ASP:OD1	1:A:606:PRO:HD2	2.20	0.41
2:B:1697:HIS:ND1	2:B:1697:HIS:N	2.67	0.41
2:B:1699:PHE:CZ	2:B:1740:ASP:OD2	2.73	0.41
2:B:1762:TYR:HB3	2:B:1764:ARG:HE	1.84	0.41
2:B:1972:LYS:HE3	2:B:1972:LYS:HB2	1.86	0.41
1:A:311:HIS:ND1	1:A:311:HIS:C	2.74	0.41
2:B:1774:THR:CG2	2:B:1814:THR:HG22	2.50	0.41
2:B:1791:SER:OG	2:B:1792:TYR:N	2.53	0.41
2:B:2295:ASN:OD1	2:B:2295:ASN:N	2.52	0.41
1:A:313:SER:OG	1:A:314:SER:N	2.53	0.41
1:A:543:LEU:HD11	1:A:642:ILE:HG21	2.02	0.41
2:B:1733:VAL:O	2:B:1850:GLY:CA	2.68	0.41
2:B:1758:LEU:HD21	2:B:1923:GLY:HA3	2.01	0.41
2:B:1790:ILE:O	2:B:1790:ILE:HG22	2.20	0.41
2:B:2002:ILE:HB	2:B:2005:HIS:HB2	2.00	0.41
2:B:2176:MET:SD	2:B:2177:PRO:HD2	2.59	0.41
2:B:2281:LYS:HE2	2:B:2282:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:HB	1:A:139:GLN:HA	2.02	0.41
1:A:200:ALA:HB3	1:A:202:PHE:HE1	1.85	0.41
2:B:1821:HIS:C	2:B:1823:MET:H	2.24	0.41
2:B:2070:TRP:HE3	2:B:2150:ARG:HD2	1.85	0.41
2:B:2246:GLN:N	2:B:2286:ASN:ND2	2.68	0.41
1:A:77:GLN:CB	1:A:177:LEU:HD12	2.44	0.41
1:A:163:ASP:HB3	1:A:166:LYS:HB3	2.01	0.41
1:A:232:HIS:CD2	1:A:318:ASP:HB2	2.56	0.41
1:A:432:THR:CB	1:A:440:GLU:HB3	2.46	0.41
1:A:8:GLY:N	1:A:52:VAL:O	2.46	0.41
1:A:197:LEU:HD11	1:A:255:TRP:CE3	2.55	0.41
1:A:200:ALA:HB1	1:A:202:PHE:CE1	2.56	0.41
1:A:422:LYS:HB2	1:A:422:LYS:HE3	1.81	0.41
2:B:1839:SER:N	2:B:1851:LEU:HD21	2.35	0.41
2:B:2302:LEU:HD22	2:B:2302:LEU:N	2.35	0.41
2:B:2304:ARG:HD2	2:B:2305:TYR:CE2	2.56	0.41
5:E:3:BMA:H61	5:E:6:MAN:H2	1.36	0.41
1:A:75:THR:CG2	1:A:175:ALA:HB3	2.27	0.41
1:A:159:LEU:HD23	1:A:159:LEU:N	2.36	0.41
1:A:574:ILE:HB	1:A:639:ILE:HG22	2.03	0.41
1:A:608:PHE:HA	1:A:611:SER:OG	2.21	0.41
1:A:309:PHE:HB2	1:A:321:GLU:HG2	2.02	0.41
1:A:387:ALA:HB2	1:A:466:LYS:HG3	2.02	0.41
2:B:1946:SER:N	2:B:1978:LEU:HD12	2.36	0.41
1:A:471:ARG:HG3	1:A:585:TRP:CZ3	2.36	0.41
1:A:527:ARG:HD2	1:A:527:ARG:H	1.86	0.41
1:A:690:LEU:HB3	1:A:708:VAL:N	2.36	0.41
1:A:690:LEU:CD2	1:A:692:CYS:HB2	2.51	0.41
1:A:698:ARG:O	1:A:699:ASN:C	2.59	0.41
1:A:708:VAL:CG1	1:A:709:SER:N	2.84	0.41
2:B:1739:THR:CB	2:B:1746:PRO:HG2	2.51	0.41
2:B:1831:ASP:OD1	2:B:1831:ASP:N	2.53	0.41
2:B:1885:GLU:HB3	2:B:1886:THR:H	1.57	0.41
2:B:1891:PHE:O	2:B:1892:THR:C	2.58	0.41
2:B:1929:LEU:HG	2:B:1930:PRO:CD	2.51	0.41
2:B:1947:MET:HE3	2:B:1947:MET:HA	2.03	0.41
2:B:1997:ARG:HG2	2:B:1999:GLU:HG2	2.02	0.41
2:B:2081:ILE:HD12	2:B:2149:ILE:CD1	2.43	0.41
2:B:2105:TYR:CD2	2:B:2144:ILE:CG2	3.04	0.41
2:B:2261:LEU:O	2:B:2309:HIS:N	2.37	0.41
1:A:232:HIS:HD2	1:A:318:ASP:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:O	1:A:235:ASN:CB	2.69	0.41
1:A:461:LEU:HD22	1:A:513:TRP:HE3	1.84	0.41
1:A:503:ILE:C	1:A:504:LEU:HD12	2.41	0.41
1:A:663:VAL:HG22	2:B:1968:LYS:NZ	2.36	0.41
2:B:1745:GLN:HA	2:B:1746:PRO:HA	1.65	0.41
2:B:1749:ARG:HH11	2:B:1749:ARG:CG	2.30	0.41
2:B:1771:ILE:HD12	2:B:1817:TRP:HE1	1.86	0.41
1:A:7:LEU:HG	1:A:8:GLY:O	2.21	0.40
1:A:163:ASP:O	1:A:167:ASP:HB2	2.21	0.40
1:A:512:LYS:HE3	1:A:514:THR:HG1	1.85	0.40
1:A:663:VAL:HG22	2:B:1968:LYS:CE	2.49	0.40
1:A:663:VAL:HG22	2:B:1968:LYS:HZ3	1.86	0.40
1:A:702:MET:O	1:A:703:THR:OG1	2.34	0.40
2:B:1730:PHE:HA	2:B:1893:GLU:OE1	2.20	0.40
2:B:1870:GLN:O	2:B:1871:VAL:HB	2.21	0.40
1:A:65:ARG:O	1:A:66:PRO:O	2.39	0.40
1:A:147:MET:CE	2:B:1972:LYS:HZ2	2.34	0.40
1:A:247:GLY:O	1:A:326:VAL:HG23	2.21	0.40
1:A:290:PRO:HG2	1:A:291:ILE:H	1.86	0.40
1:A:470:SER:HB3	1:A:471:ARG:H	1.64	0.40
1:A:476:TYR:HA	1:A:477:PRO:HD3	1.97	0.40
1:A:683:GLU:HB2	1:A:685:PRO:HD2	2.03	0.40
2:B:1849:SER:OG	2:B:1888:SER:C	2.59	0.40
2:B:2048:PRO:CG	2:B:2062:TRP:CD1	2.94	0.40
2:B:2242:GLY:HA2	2:B:2297:LEU:HD12	2.03	0.40
2:B:2274:PHE:CD1	2:B:2274:PHE:C	2.95	0.40
2:B:2322:GLU:HG3	2:B:2323:VAL:O	2.20	0.40
1:A:3:ARG:HH12	1:A:79:GLU:HG2	1.86	0.40
1:A:8:GLY:HA3	1:A:52:VAL:HG22	2.02	0.40
1:A:105:TYR:HB3	1:A:109:SER:CB	2.22	0.40
1:A:238:VAL:N	1:A:241:SER:OG	2.54	0.40
1:A:376:LYS:C	1:A:377:LYS:HG2	2.42	0.40
1:A:400:LEU:HD23	1:A:400:LEU:N	2.36	0.40
1:A:432:THR:CG2	1:A:433:ASP:OD1	2.70	0.40
1:A:526:PRO:HB2	1:A:679:PHE:CZ	2.56	0.40
2:B:1699:PHE:HD1	2:B:1774:THR:OG1	2.05	0.40
2:B:1739:THR:CB	2:B:1746:PRO:CG	2.99	0.40
2:B:1831:ASP:O	2:B:1858:CYS:CB	2.66	0.40
2:B:1927:ASP:OD1	2:B:2011:SER:O	2.39	0.40
2:B:2236:LYS:HB3	2:B:2330:ASP:OD1	2.21	0.40
1:A:114:TYR:N	1:A:114:TYR:CD1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:O	1:A:696:ASP:N	2.54	0.40
2:B:1759:LEU:HD11	2:B:1879:PHE:HB3	2.03	0.40
2:B:2032:ILE:HA	2:B:2036:GLN:HE22	1.85	0.40
2:B:2035:PHE:CE1	2:B:2036:GLN:HG3	2.57	0.40
2:B:2059:ILE:HG13	2:B:2059:ILE:O	2.21	0.40
2:B:2166:LEU:H	2:B:2166:LEU:HG	1.66	0.40
1:A:56:ASP:O	1:A:57:HIS:CB	2.66	0.40
1:A:100:ALA:O	1:A:101:VAL:C	2.59	0.40
1:A:237:TYR:CD1	1:A:242:LEU:HD22	2.57	0.40
1:A:386:ILE:CD1	1:A:428:PHE:HD2	2.31	0.40
1:A:663:VAL:HG13	2:B:1968:LYS:CG	2.52	0.40
2:B:1784:SER:HB3	2:B:1840:ASP:OD1	2.21	0.40
2:B:1819:VAL:HA	2:B:1823:MET:HE1	2.01	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:NH1	1:A:496:LYS:NZ[7_555]	1.94	0.26

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	599/740 (81%)	448 (75%)	111 (18%)	40 (7%)	1 18
2	B	613/865 (71%)	498 (81%)	87 (14%)	28 (5%)	2 24
All	All	1212/1605 (76%)	946 (78%)	198 (16%)	68 (6%)	2 21

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	TRP
1	A	127	LYS
1	A	229	PRO
1	A	243	PRO
1	A	312	ILE
1	A	437	LYS
1	A	492	PRO
1	A	497	HIS
1	A	621	VAL
1	A	646	THR
1	A	663	VAL
1	A	705	LEU
1	A	713	LYS
2	B	1740	ASP
2	B	1768	GLU
2	B	1841	VAL
2	B	1871	VAL
2	B	1886	THR
2	B	1930	PRO
2	B	1984	GLU
2	B	2158	ILE
1	A	403	ASP
1	A	695	SER
1	A	706	LEU
2	B	1935	ALA
2	B	2049	LYS
2	B	2170	ASP
1	A	66	PRO
1	A	159	LEU
1	A	434	GLU
1	A	501	PHE
1	A	539	MET
1	A	618	ASN
1	A	658	PHE
2	B	1695	THR
2	B	1909	ASP
2	B	2052	ARG
1	A	153	CYS
1	A	163	ASP
1	A	264	PRO
1	A	284	ALA
1	A	397	PRO
2	B	1746	PRO

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Mol	Chain	Res	Type
2	B	1830	PHE
2	B	1908	GLU
2	B	1922	ASN
2	B	1967	LYS
1	A	410	GLN
1	A	601	VAL
1	A	674	SER
1	A	689	ILE
2	B	1854	PRO
2	B	2200	PHE
2	B	2273	LEU
2	B	2286	ASN
1	A	684	ASN
1	A	699	ASN
2	B	1752	LEU
2	B	1926	MET
2	B	2299	PRO
1	A	502	PRO
1	A	103	VAL
1	A	550	PRO
1	A	378	HIS
1	A	546	GLY
2	B	2135	ILE
2	B	2292	PRO
1	A	242	LEU

5.3.2 Protein sidechains (i)

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	542/660 (82%)	415 (77%)	127 (23%)	1 5
2	B	550/776 (71%)	413 (75%)	137 (25%)	0 4
All	All	1092/1436 (76%)	828 (76%)	264 (24%)	0 5

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	55	THR
1	A	76	ILE
1	A	82	ASP
1	A	84	VAL
1	A	94	HIS
1	A	99	HIS
1	A	105	TYR
1	A	106	TRP
1	A	114	TYR
1	A	120	GLN
1	A	127	LYS
1	A	129	PHE
1	A	138	TRP
1	A	142	LYS
1	A	147	MET
1	A	149	SER
1	A	152	LEU
1	A	154	LEU
1	A	177	LEU
1	A	194	LYS
1	A	198	LEU
1	A	201	VAL
1	A	230	LYS
1	A	233	THR
1	A	235	ASN
1	A	241	SER
1	A	242	LEU
1	A	260	MET
1	A	279	ARG
1	A	291	ILE
1	A	292	THR
1	A	295	THR
1	A	299	LEU
1	A	302	ASP
1	A	306	PHE
1	A	309	PHE
1	A	311	HIS
1	A	318	ASP
1	A	328	SER
1	A	331	GLU
1	A	376	LYS
1	A	381	THR

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Mol	Chain	Res	Type
1	A	382	TRP
1	A	383	VAL
1	A	386	ILE
1	A	392	ASP
1	A	393	TRP
1	A	398	LEU
1	A	400	LEU
1	A	403	ASP
1	A	404	ASP
1	A	410	GLN
1	A	412	LEU
1	A	413	ASN
1	A	421	ARG
1	A	426	VAL
1	A	431	TYR
1	A	433	ASP
1	A	437	LYS
1	A	448	ILE
1	A	453	LEU
1	A	454	TYR
1	A	457	VAL
1	A	460	THR
1	A	470	SER
1	A	471	ARG
1	A	475	ILE
1	A	481	THR
1	A	486	LEU
1	A	496	LYS
1	A	498	LEU
1	A	499	LYS
1	A	500	ASP
1	A	503	ILE
1	A	504	LEU
1	A	509	PHE
1	A	514	THR
1	A	516	THR
1	A	517	VAL
1	A	518	GLU
1	A	523	LYS
1	A	524	SER
1	A	525	ASP
1	A	527	ARG

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Mol	Chain	Res	Type
1	A	529	LEU
1	A	531	ARG
1	A	536	PHE
1	A	538	ASN
1	A	539	MET
1	A	540	GLU
1	A	545	SER
1	A	552	LEU
1	A	555	TYR
1	A	571	ARG
1	A	573	VAL
1	A	575	LEU
1	A	578	VAL
1	A	588	THR
1	A	593	ARG
1	A	601	VAL
1	A	603	LEU
1	A	604	GLU
1	A	611	SER
1	A	618	ASN
1	A	620	TYR
1	A	624	SER
1	A	629	VAL
1	A	636	TYR
1	A	648	PHE
1	A	659	LYS
1	A	663	VAL
1	A	664	TYR
1	A	668	LEU
1	A	673	PHE
1	A	680	MET
1	A	683	GLU
1	A	684	ASN
1	A	687	LEU
1	A	688	TRP
1	A	690	LEU
1	A	698	ARG
1	A	699	ASN
1	A	705	LEU
1	A	708	VAL
1	A	709	SER
1	A	713	LYS

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Mol	Chain	Res	Type
2	B	1694	LYS
2	B	1695	THR
2	B	1696	ARG
2	B	1697	HIS
2	B	1700	ILE
2	B	1705	ARG
2	B	1707	TRP
2	B	1708	ASP
2	B	1711	MET
2	B	1726	SER
2	B	1733	VAL
2	B	1747	LEU
2	B	1749	ARG
2	B	1752	LEU
2	B	1756	LEU
2	B	1758	LEU
2	B	1759	LEU
2	B	1767	VAL
2	B	1769	ASP
2	B	1780	SER
2	B	1781	ARG
2	B	1786	TYR
2	B	1797	ARG
2	B	1804	LYS
2	B	1810	ASN
2	B	1814	THR
2	B	1827	LYS
2	B	1828	ASP
2	B	1831	ASP
2	B	1843	LEU
2	B	1846	ASP
2	B	1849	SER
2	B	1851	LEU
2	B	1856	LEU
2	B	1857	VAL
2	B	1859	HIS
2	B	1862	THR
2	B	1863	LEU
2	B	1867	HIS
2	B	1869	ARG
2	B	1879	PHE
2	B	1882	ILE

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Mol	Chain	Res	Type
2	B	1889	TRP
2	B	1890	TYR
2	B	1891	PHE
2	B	1914	GLU
2	B	1928	THR
2	B	1934	MET
2	B	1938	GLN
2	B	1944	LEU
2	B	1945	LEU
2	B	1946	SER
2	B	1947	MET
2	B	1951	GLU
2	B	1952	ASN
2	B	1953	ILE
2	B	1964	THR
2	B	1967	LYS
2	B	1973	MET
2	B	1975	LEU
2	B	1977	ASN
2	B	1978	LEU
2	B	1984	GLU
2	B	1989	LEU
2	B	1995	ILE
2	B	1997	ARG
2	B	1999	GLU
2	B	2004	GLU
2	B	2013	LEU
2	B	2015	LEU
2	B	2022	GLN
2	B	2027	MET
2	B	2034	ASP
2	B	2035	PHE
2	B	2037	ILE
2	B	2040	SER
2	B	2042	GLN
2	B	2049	LYS
2	B	2068	PHE
2	B	2076	LEU
2	B	2079	MET
2	B	2081	ILE
2	B	2090	ARG
2	B	2091	GLN

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Mol	Chain	Res	Type
2	B	2095	SER
2	B	2096	LEU
2	B	2098	ILE
2	B	2101	PHE
2	B	2102	ILE
2	B	2111	LYS
2	B	2114	THR
2	B	2116	ARG
2	B	2120	THR
2	B	2123	LEU
2	B	2129	ASN
2	B	2135	ILE
2	B	2139	ILE
2	B	2145	ILE
2	B	2154	THR
2	B	2156	TYR
2	B	2157	SER
2	B	2165	GLU
2	B	2166	LEU
2	B	2171	LEU
2	B	2175	SER
2	B	2178	LEU
2	B	2186	SER
2	B	2195	TYR
2	B	2199	MET
2	B	2204	SER
2	B	2206	SER
2	B	2212	LEU
2	B	2213	GLN
2	B	2220	ARG
2	B	2232	VAL
2	B	2237	THR
2	B	2243	VAL
2	B	2245	THR
2	B	2246	GLN
2	B	2249	LYS
2	B	2261	LEU
2	B	2262	ILE
2	B	2269	HIS
2	B	2275	PHE
2	B	2280	VAL
2	B	2281	LYS

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Mol	Chain	Res	Type
2	B	2290	PHE
2	B	2295	ASN
2	B	2297	LEU
2	B	2301	LEU
2	B	2302	LEU
2	B	2304	ARG
2	B	2306	LEU
2	B	2307	ARG
2	B	2326	CYS
2	B	2331	LEU
2	B	2332	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	232	HIS
1	A	615	HIS
1	A	684	ASN
2	B	2287	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)

13 monosaccharides 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	$\#\|Z\| > 2$
3	NAG	C	1	3,1	14,14,15	0.45	0	17,19,21	0.74	0
3	NAG	C	2	3	14,14,15	0.38	0	17,19,21	1.27	1 (5%)
3	BMA	C	3	3	11,11,12	0.34	0	15,15,17	1.84	3 (20%)
3	MAN	C	4	3	11,11,12	0.29	0	15,15,17	0.94	1 (6%)
4	NAG	D	1	4,2	14,14,15	0.63	0	17,19,21	1.48	2 (11%)
4	NAG	D	2	4	14,14,15	0.43	0	17,19,21	1.70	5 (29%)
5	NAG	E	1	5,2	14,14,15	0.51	0	17,19,21	2.48	5 (29%)
5	NAG	E	2	5	14,14,15	0.55	0	17,19,21	1.41	3 (17%)
5	BMA	E	3	5	11,11,12	0.58	0	15,15,17	1.08	1 (6%)
5	BMA	E	4	5	11,11,12	0.28	0	15,15,17	0.76	0
5	MAN	E	5	5	11,11,12	0.27	0	15,15,17	0.57	0
5	MAN	E	6	5	11,11,12	0.62	0	15,15,17	1.38	2 (13%)
5	MAN	E	7	5	11,11,12	0.48	0	15,15,17	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
5	NAG	E	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	BMA	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1	NAG	O5-C5-C6	5.68	116.11	107.20
5	E	1	NAG	C2-N2-C7	5.50	130.73	122.90
3	C	3	BMA	C1-C2-C3	5.19	116.05	109.67
3	C	2	NAG	O5-C5-C6	3.88	113.28	107.20
4	D	2	NAG	C4-C3-C2	3.78	116.56	111.02
4	D	2	NAG	C3-C4-C5	3.53	116.54	110.24
5	E	1	NAG	C3-C4-C5	3.40	116.30	110.24
3	C	3	BMA	O5-C1-C2	3.38	115.98	110.77
5	E	6	MAN	C1-C2-C3	3.37	113.81	109.67
5	E	1	NAG	C1-C2-N2	3.17	115.90	110.49
4	D	1	NAG	C2-N2-C7	3.06	127.27	122.90
5	E	6	MAN	C1-O5-C5	3.04	116.31	112.19
5	E	2	NAG	O5-C5-C4	-2.83	103.94	110.83
5	E	2	NAG	C2-N2-C7	2.82	126.92	122.90
4	D	1	NAG	O5-C5-C6	2.80	111.59	107.20
5	E	3	BMA	C1-O5-C5	2.63	115.76	112.19
3	C	4	MAN	C1-C2-C3	2.54	112.78	109.67
5	E	2	NAG	C6-C5-C4	2.39	118.61	113.00
4	D	2	NAG	O5-C1-C2	-2.30	107.65	111.29
5	E	1	NAG	O5-C1-C2	2.23	114.82	111.29
3	C	3	BMA	C1-O5-C5	2.20	115.17	112.19
4	D	2	NAG	C2-N2-C7	2.19	126.02	122.90
4	D	2	NAG	C8-C7-N2	2.12	119.70	116.10

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	3	BMA	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

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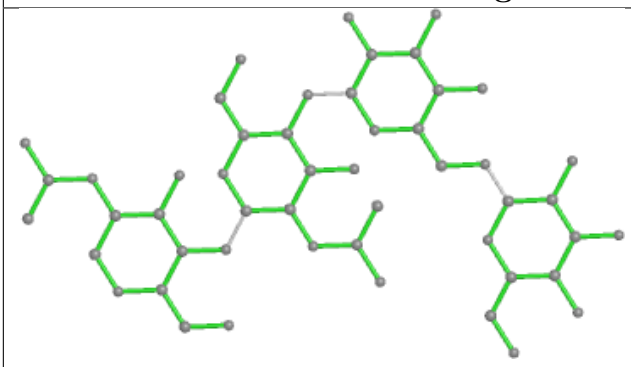
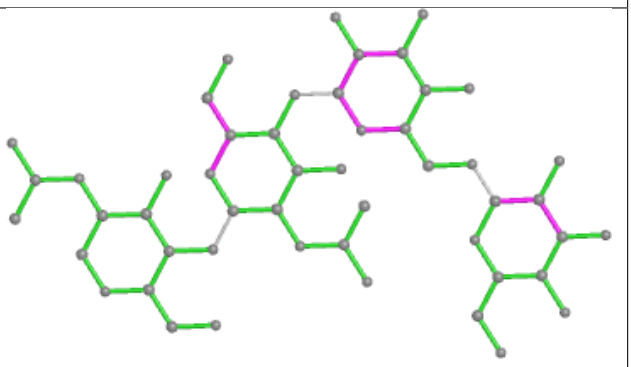
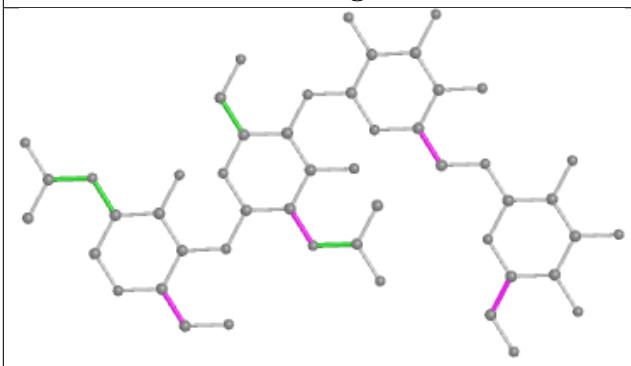
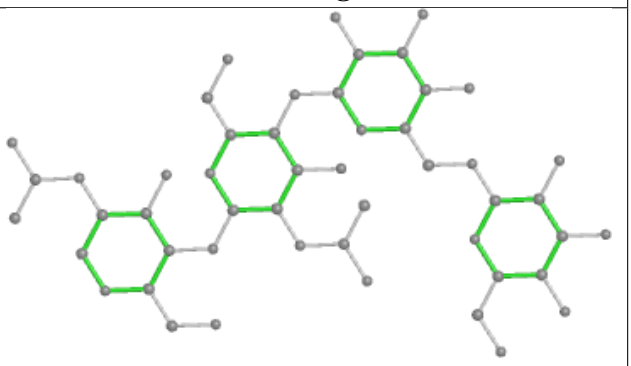
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	C	3	BMA	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6

There are no ring outliers.

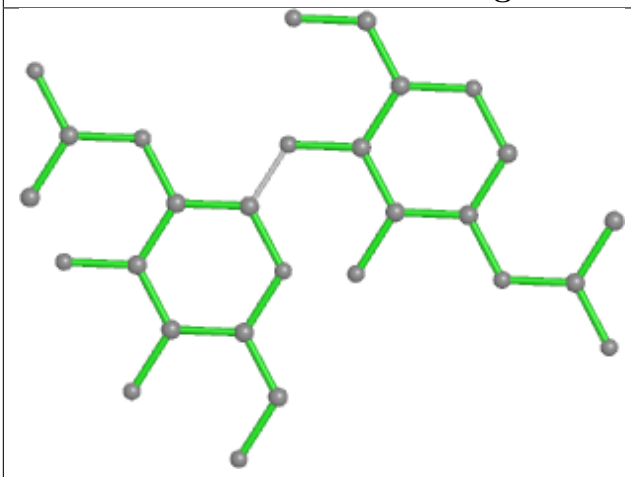
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	7	MAN	1	0
3	C	1	NAG	1	0
5	E	2	NAG	1	0
5	E	6	MAN	2	0
3	C	3	BMA	7	0
3	C	4	MAN	4	0
5	E	3	BMA	3	0
3	C	2	NAG	4	0
5	E	5	MAN	1	0

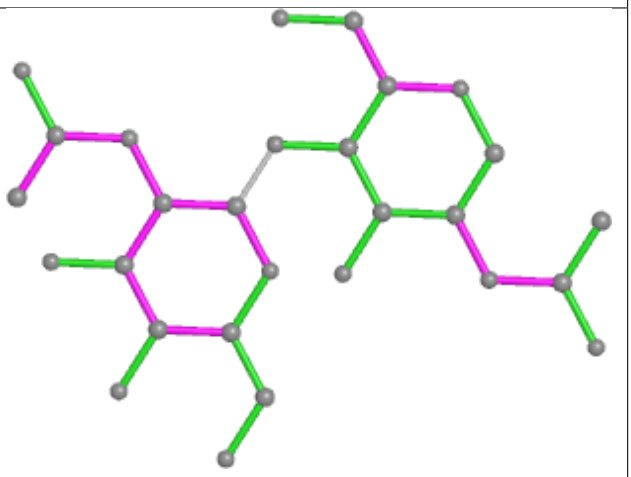
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C	
 Bond lengths	 Bond angles
 Torsions	 Rings

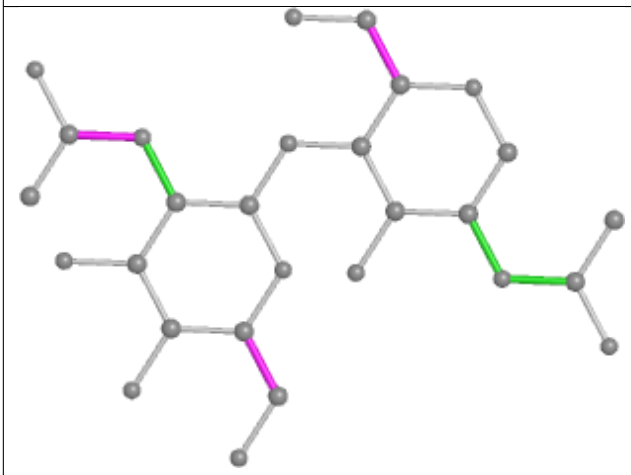
Oligosaccharide Chain D



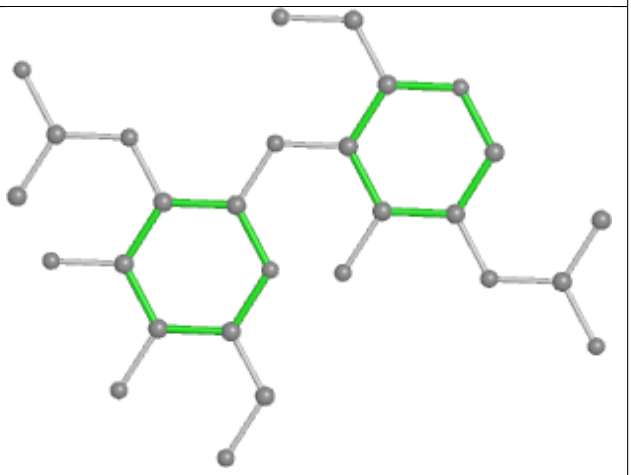
Bond lengths



Bond angles

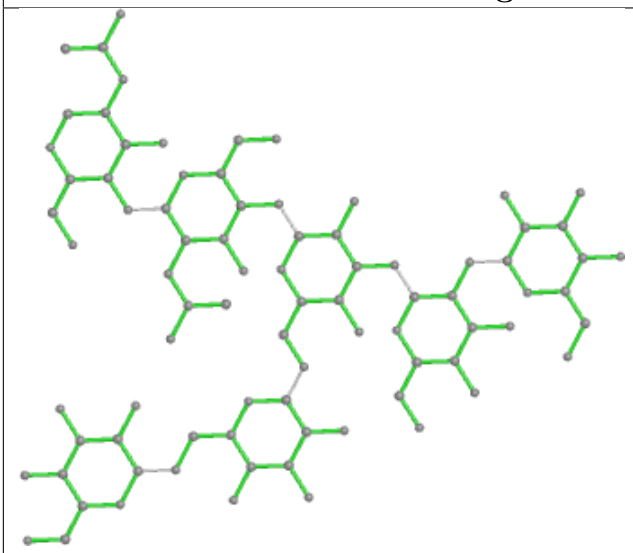


Torsions

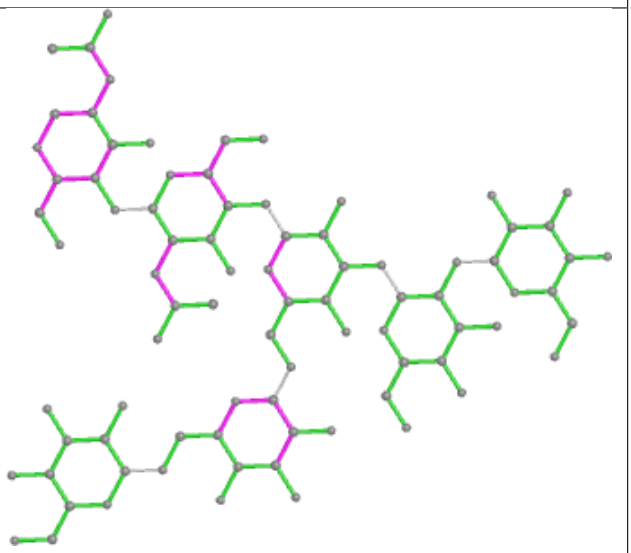


Rings

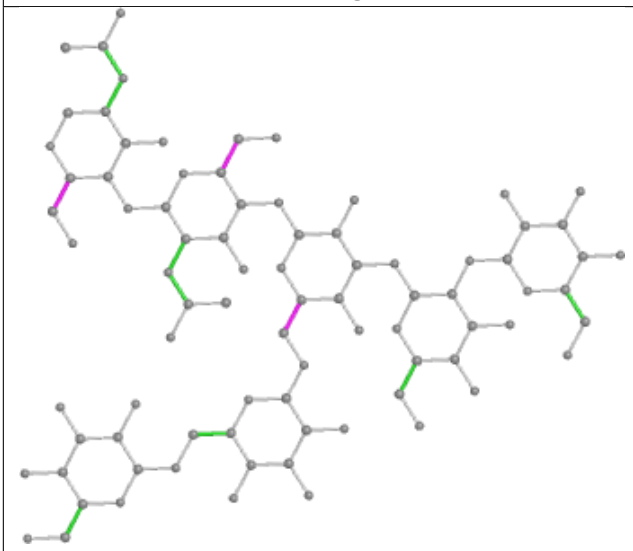
Oligosaccharide Chain E



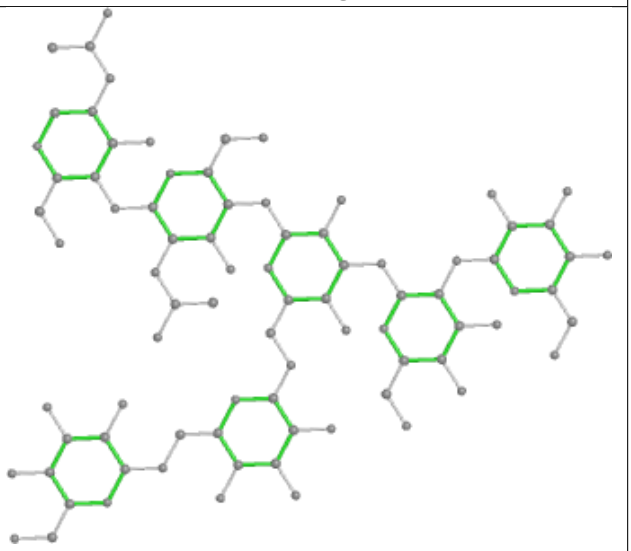
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	611/740 (82%)	-0.42	1 (0%)	95	93	99, 186, 319, 397	0
2	B	619/865 (71%)	-0.36	3 (0%)	91	86	106, 195, 319, 424	0
All	All	1230/1605 (76%)	-0.39	4 (0%)	94	90	99, 191, 319, 424	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2058	SER	2.4
1	A	190	GLN	2.3
2	B	1744	THR	2.3
2	B	1743	PHE	2.1

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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	2	14/15	0.64	0.42	307,363,404,410	0
5	BMA	E	3	11/12	0.69	0.23	278,295,314,335	0
4	NAG	D	1	14/15	0.70	0.45	275,361,420,429	0
5	MAN	E	7	11/12	0.74	0.32	303,330,373,383	0
3	MAN	C	4	11/12	0.78	0.17	193,218,224,226	11

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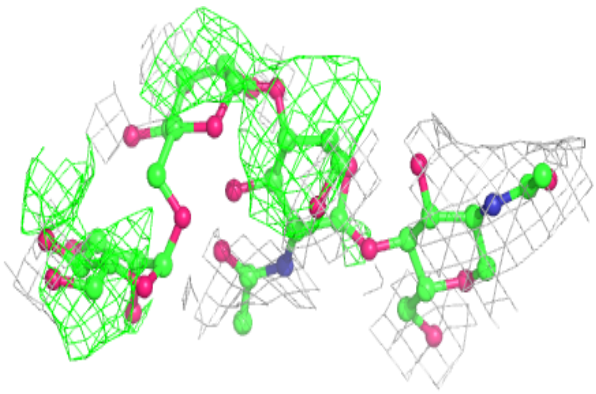
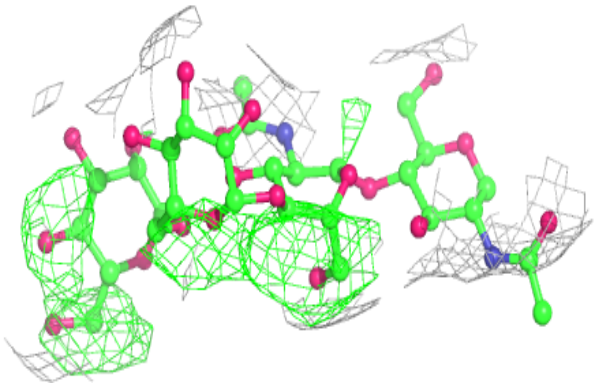
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	C	3	11/12	0.81	0.14	181,207,223,224	11
5	MAN	E	5	11/12	0.82	0.27	192,215,228,233	11
3	NAG	C	2	14/15	0.85	0.12	169,231,241,258	14
3	NAG	C	1	14/15	0.85	0.25	199,244,264,269	0
5	MAN	E	6	11/12	0.87	0.22	348,364,380,392	0
5	BMA	E	4	11/12	0.90	0.17	222,241,252,258	11
5	NAG	E	1	14/15	0.92	0.26	151,202,230,232	0
5	NAG	E	2	14/15	0.94	0.39	228,247,271,273	0

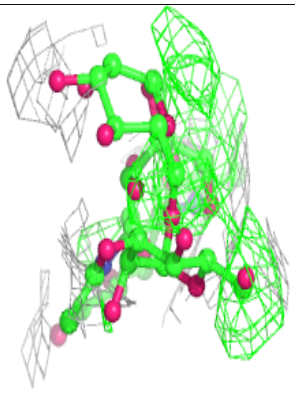
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

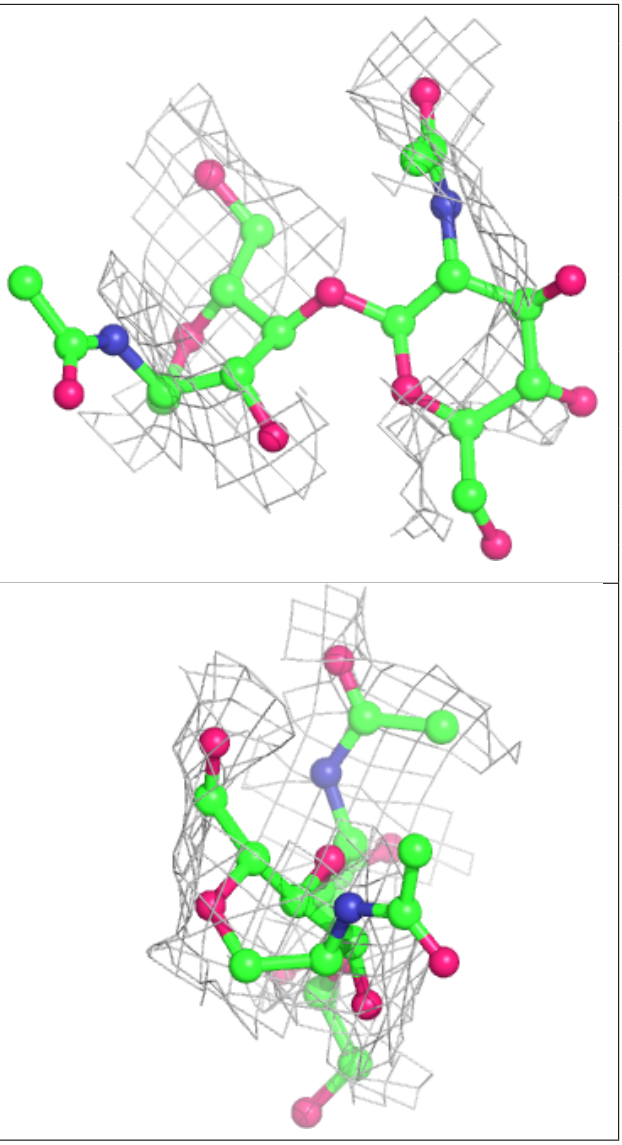






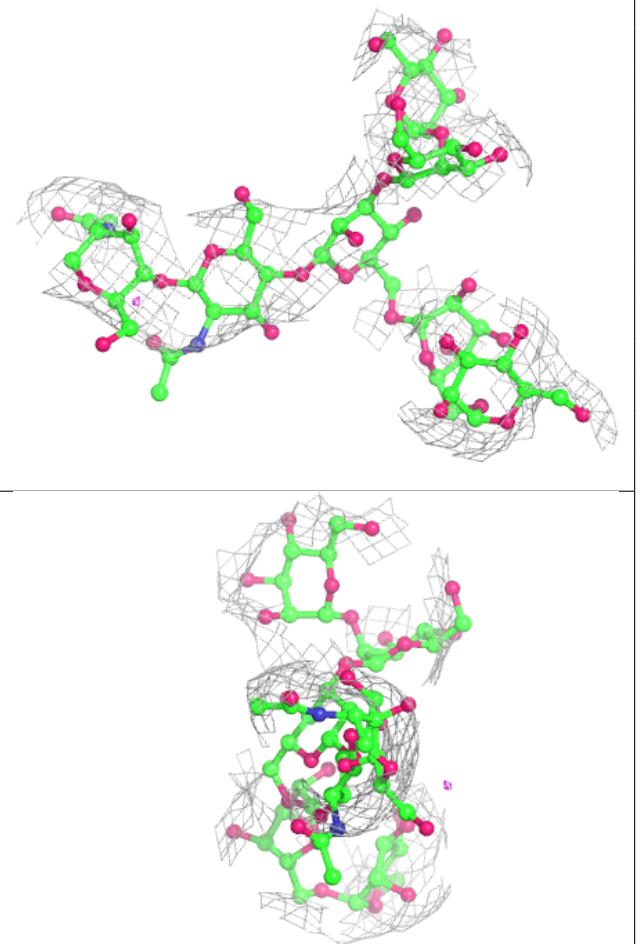
Electron density around Chain D:

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



Electron density around Chain E:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	A	806	1/1	0.93	0.21	236,236,236,236	0
7	CU	A	808	1/1	0.98	0.11	167,167,167,167	0
6	CA	A	807	1/1	0.99	0.14	165,165,165,165	0
6	CA	A	805	1/1	0.99	0.14	215,215,215,215	0
7	CU	B	2610	1/1	0.99	0.12	150,150,150,150	0

6.5 Other polymers (i)

There are no such residues in this entry.