



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:13 AM UTC

PDB ID : 4BDV / pdb_00004bdv
Title : CRYSTAL STRUCTURE OF A TRUNCATED B-DOMAIN HUMAN FACTOR VIII
Authors : Svensson, L.A.; Thim, L.; Olsen, O.H.; Nicolaisen, E.M.
Deposited on : 2012-10-08
Resolution : 3.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

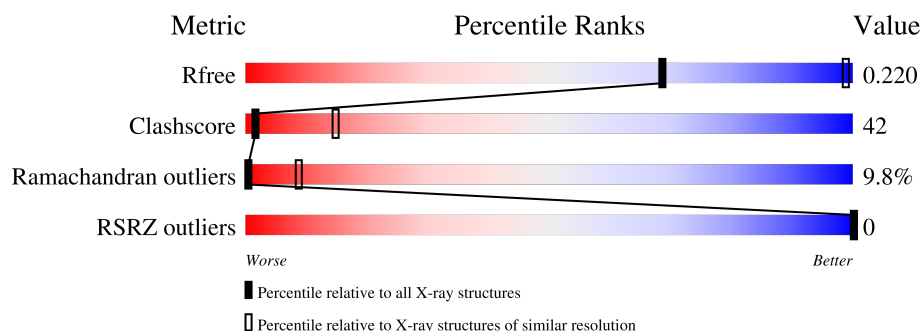
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
RSRZ outliers	180081	1016 (4.18-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	760	29% 40% 11% • 19%
2	B	685	35% 45% 8% • 12%
3	C	2	50% 50%
4	D	5	20% 80%

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	NAG	C	1	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9973 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 FACTOR VIIIA HEAVY CHAIN, 92 KDA ISOFORM, B DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4944	3194	826	900	24			

- Molecule 2 is a protein called FACTOR VIIIA LIGHT CHAIN.

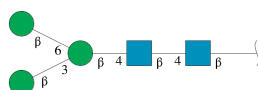
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	606	Total	C	N	O	S	0	0	0
			4929	3175	841	885	28			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

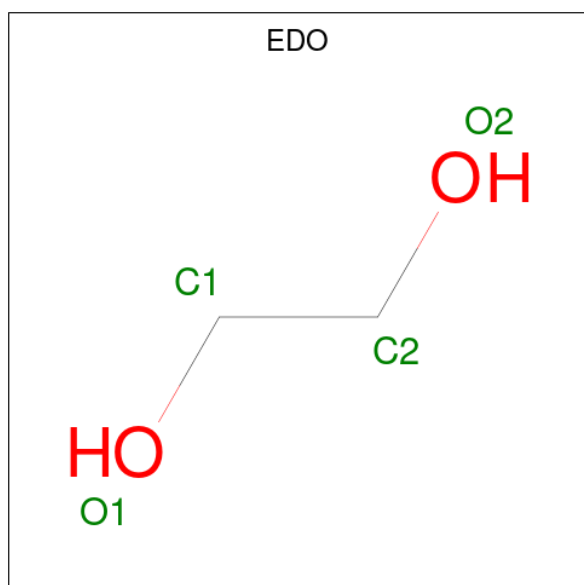
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

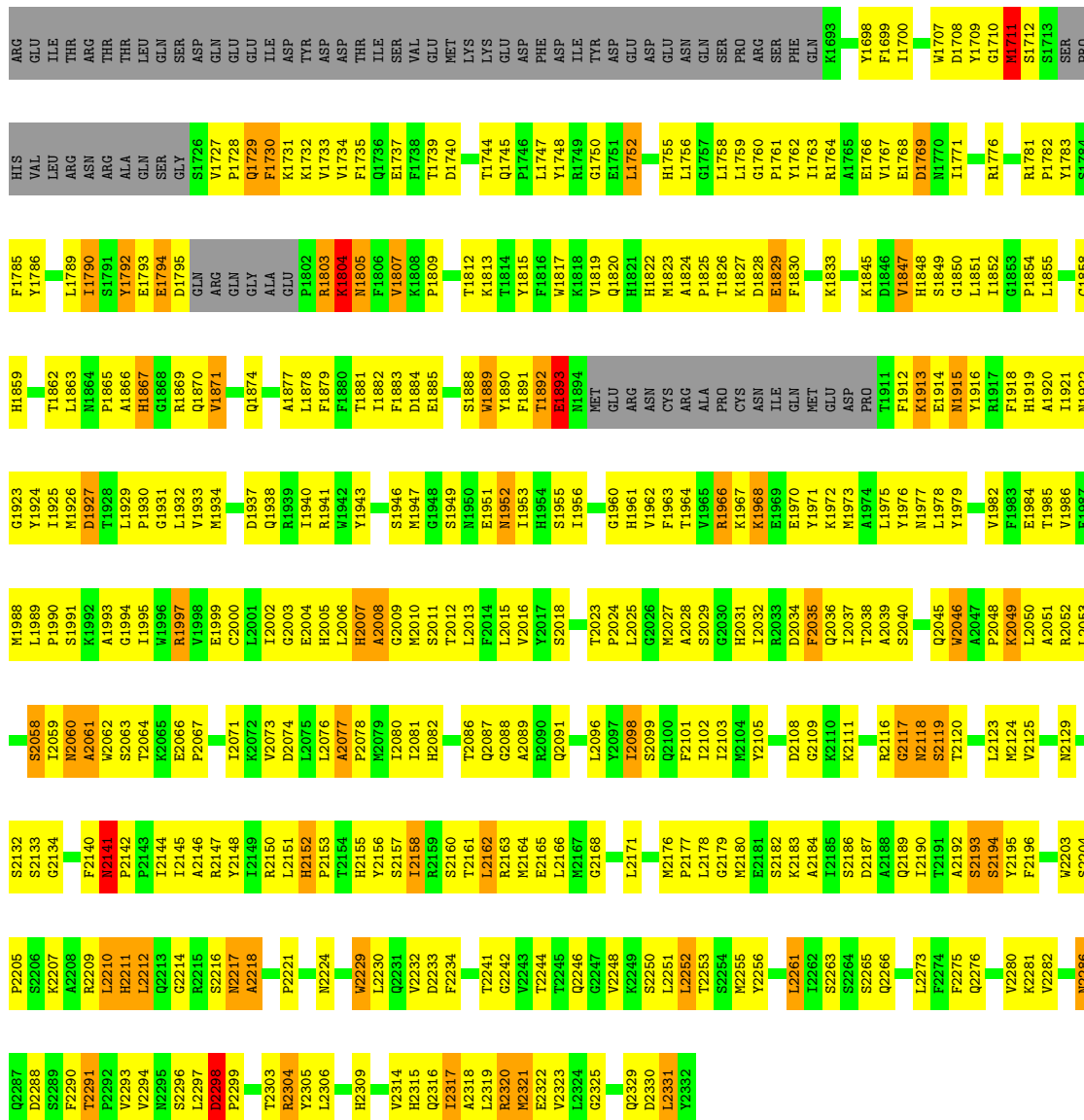
- Molecule 8 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cu	0	0
			1	1		

ARG
HIS
PRO
SER
GLN
ASN
PRO
PRO
VAL
LEU
LYS
ARG
HIS
GLN

● Molecule 2: FACTOR VIIIA LIGHT CHAIN

Chain B: 35% 45% 8% 12%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%

NAG1
NAG2

- Molecule 4: beta-D-mannopyranose-(1-3)-[beta-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

se



MAG1
MAG2
BMA3
BMA4
BMA5

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.84Å 133.84Å 355.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.98 20.00 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.98) 98.9 (20.00-3.98)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.94Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.162 , 0.246 (Not available) , 0.220	Depositor DCC
R_{free} test set	1458 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	134.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 125.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9973	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ZN, CU1, BMA, NAG, CA

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	0.94	10/5085 (0.2%)	1.38	74/6901 (1.1%)
2	B	0.88	6/5070 (0.1%)	1.29	53/6864 (0.8%)
All	All	0.91	16/10155 (0.2%)	1.34	127/13765 (0.9%)

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	5
2	B	0	3
All	All	0	8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	TYR	N-CA	8.81	1.57	1.46
1	A	230	LYS	N-CA	7.57	1.55	1.46
1	A	45	VAL	CA-C	6.98	1.61	1.52
1	A	230	LYS	CA-C	6.94	1.62	1.52
2	B	1804	LYS	CA-C	6.25	1.61	1.52
2	B	1727	VAL	N-CA	5.97	1.53	1.46
1	A	48	LYS	CA-C	5.83	1.60	1.52
1	A	232	HIS	N-CA	5.61	1.53	1.46
2	B	1804	LYS	N-CA	5.57	1.53	1.46
2	B	1728	PRO	N-CA	5.44	1.53	1.47
1	A	61	ILE	CA-CB	5.34	1.60	1.54
1	A	60	ASN	N-CA	5.32	1.52	1.45
2	B	1727	VAL	CA-C	5.25	1.58	1.52
2	B	1916	TYR	N-CA	5.15	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	THR	N-CA	5.15	1.52	1.46
1	A	46	TYR	CA-C	5.07	1.59	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1727	VAL	CA-C-N	12.91	133.06	119.76
2	B	1727	VAL	C-N-CA	12.91	133.06	119.76
1	A	60	ASN	N-CA-C	10.31	125.84	109.86
1	A	46	TYR	N-CA-C	9.92	131.93	110.80
2	B	1728	PRO	N-CA-C	9.26	125.59	111.14
1	A	313	SER	N-CA-C	9.11	120.90	110.97
1	A	15	ASP	N-CA-C	9.09	130.16	110.80
1	A	495	VAL	N-CA-C	8.77	120.26	109.30
1	A	48	LYS	N-CA-C	8.73	121.17	108.86
1	A	14	TRP	N-CA-C	8.65	123.27	110.46
1	A	597	ASN	CA-C-N	8.35	130.28	119.84
1	A	597	ASN	C-N-CA	8.35	130.28	119.84
2	B	1824	ALA	CA-C-N	8.04	128.34	119.90
2	B	1824	ALA	C-N-CA	8.04	128.34	119.90
1	A	399	VAL	N-CA-C	7.76	119.08	107.51
1	A	150	ASP	CA-C-N	7.70	129.46	119.84
1	A	150	ASP	C-N-CA	7.70	129.46	119.84
1	A	475	ILE	N-CA-C	7.67	118.95	107.75
1	A	666	ASP	N-CA-C	-7.63	103.82	113.43
2	B	2304	ARG	N-CA-C	-7.61	104.89	114.56
1	A	230	LYS	N-CA-C	7.59	126.97	110.80
2	B	2141	ASN	O-C-N	7.56	126.35	120.38
1	A	66	PRO	CA-C-N	7.55	129.28	119.84
1	A	66	PRO	C-N-CA	7.55	129.28	119.84
1	A	208	TRP	N-CA-C	-7.43	101.33	112.54
2	B	1727	VAL	N-CA-C	7.42	124.91	108.88
1	A	286	LEU	N-CA-C	-7.28	98.75	110.32
1	A	682	MET	N-CA-C	7.25	119.47	109.54
2	B	1847	VAL	N-CA-C	-7.18	105.94	111.62
1	A	194	LYS	N-CA-C	7.04	121.16	108.69
1	A	693	HIS	CB-CA-C	7.04	119.95	111.22
1	A	684	ASN	CA-C-N	7.03	126.96	120.21
1	A	684	ASN	C-N-CA	7.03	126.96	120.21
2	B	2125	VAL	CB-CA-C	-6.96	102.28	110.91
2	B	1792	TYR	N-CA-C	6.90	119.91	109.63
1	A	486	LEU	N-CA-C	6.89	118.44	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	SER	CA-C-N	6.85	128.40	119.84
1	A	289	SER	C-N-CA	6.85	128.40	119.84
1	A	65	ARG	N-CA-C	6.66	118.04	109.72
2	B	2298	ASP	CA-C-N	-6.64	113.54	120.38
2	B	2298	ASP	C-N-CA	-6.64	113.54	120.38
1	A	534	SER	N-CA-C	6.58	116.96	108.34
1	A	324	VAL	CB-CA-C	-6.52	101.11	110.83
1	A	501	PHE	CA-C-N	6.52	129.05	120.25
1	A	501	PHE	C-N-CA	6.52	129.05	120.25
1	A	233	THR	N-CA-C	6.51	120.25	109.96
1	A	474	ASN	N-CA-C	6.46	117.66	108.74
2	B	2217	ASN	N-CA-C	6.44	117.62	108.54
2	B	2261	LEU	CA-CB-CG	-6.40	93.89	116.30
1	A	444	HIS	N-CA-C	-6.35	104.36	111.28
1	A	441	ALA	N-CA-C	6.34	119.67	110.28
2	B	1805	ASN	N-CA-C	6.33	118.15	108.52
1	A	181	GLU	N-CA-C	6.29	120.51	112.34
2	B	1803	ARG	N-CA-C	6.25	119.38	107.75
2	B	2190	ILE	CB-CA-C	-6.18	102.08	110.42
1	A	572	ASN	N-CA-C	6.15	118.81	107.99
2	B	1927	ASP	N-CA-C	6.06	120.67	113.16
2	B	2152	HIS	CA-C-N	6.05	125.81	119.76
2	B	2152	HIS	C-N-CA	6.05	125.81	119.76
2	B	1711	MET	N-CA-C	6.05	123.69	110.80
2	B	1769	ASP	N-CA-C	6.04	117.69	110.19
2	B	1997	ARG	N-CA-C	5.98	119.31	109.85
1	A	407	TYR	N-CA-C	-5.95	106.63	114.31
1	A	679	PHE	N-CA-C	5.94	118.12	108.26
2	B	2211	HIS	CB-CA-C	5.91	118.60	109.03
2	B	2320	ARG	N-CA-C	-5.90	101.72	110.46
1	A	584	SER	N-CA-C	-5.87	103.19	110.41
1	A	700	ARG	N-CA-C	-5.85	104.54	112.26
1	A	45	VAL	CA-C-N	5.84	132.70	121.54
1	A	45	VAL	C-N-CA	5.84	132.70	121.54
1	A	591	ILE	N-CA-CB	5.83	117.37	110.55
2	B	2103	ILE	N-CA-C	5.83	116.51	108.12
1	A	710	SER	N-CA-C	5.80	118.66	109.96
2	B	2210	LEU	CA-C-N	-5.78	112.43	122.36
2	B	2210	LEU	C-N-CA	-5.78	112.43	122.36
2	B	2040	SER	N-CA-C	-5.77	105.13	111.82
1	A	296	ALA	N-CA-C	5.77	118.17	109.23
1	A	53	GLU	N-CA-C	5.76	118.67	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1807	VAL	N-CA-C	5.75	116.14	107.80
1	A	383	VAL	N-CA-C	5.74	116.13	107.75
1	A	200	ALA	N-CA-C	5.71	118.03	108.96
1	A	126	ASP	N-CA-C	5.68	119.31	112.38
2	B	1956	ILE	N-CA-C	5.67	116.74	108.58
2	B	2134	GLY	N-CA-C	-5.66	106.11	112.33
2	B	1893	GLU	N-CA-C	5.65	122.83	110.80
1	A	709	SER	N-CA-C	5.64	117.64	109.07
1	A	50	LEU	N-CA-C	5.60	117.31	108.96
1	A	450	GLY	CA-C-N	5.60	125.91	119.92
1	A	450	GLY	C-N-CA	5.60	125.91	119.92
2	B	2060	ASN	N-CA-C	5.55	117.53	108.76
1	A	681	SER	N-CA-C	-5.54	99.01	110.80
1	A	295	THR	CB-CA-C	5.49	118.59	110.14
2	B	2007	HIS	N-CA-C	-5.47	105.76	113.20
1	A	670	LEU	N-CA-C	5.46	118.67	107.69
2	B	2317	ILE	N-CA-CB	5.45	116.47	110.53
2	B	1731	LYS	N-CA-C	-5.45	101.30	109.15
1	A	45	VAL	N-CA-C	5.40	120.57	109.34
2	B	2282	VAL	CB-CA-C	-5.38	104.94	111.88
1	A	470	SER	N-CA-C	5.32	119.49	112.89
1	A	283	GLN	N-CA-C	-5.29	100.28	108.90
1	A	3	ARG	N-CA-C	5.28	118.81	107.67
2	B	2018	SER	N-CA-C	-5.26	101.96	110.32
2	B	2058	SER	N-CA-C	-5.26	106.87	113.28
2	B	1852	ILE	CB-CA-C	-5.25	101.31	110.71
2	B	2325	GLY	N-CA-C	5.25	117.00	110.29
2	B	1962	VAL	CB-CA-C	-5.24	104.02	111.19
1	A	694	ASN	N-CA-C	-5.21	100.82	109.46
1	A	458	GLY	CA-C-N	5.14	128.38	120.82
1	A	458	GLY	C-N-CA	5.14	128.38	120.82
1	A	4	ARG	N-CA-C	5.12	117.91	109.76
2	B	1916	TYR	N-CA-C	5.11	121.69	110.80
2	B	1877	ALA	N-CA-C	5.09	117.92	107.69
1	A	396	ALA	CA-C-N	5.08	126.19	119.84
1	A	396	ALA	C-N-CA	5.08	126.19	119.84
1	A	541	ARG	N-CA-C	-5.08	105.63	111.07
1	A	646	THR	N-CA-C	5.07	121.60	110.80
2	B	2229	TRP	N-CA-C	5.07	116.00	108.60
2	B	2162	LEU	N-CA-C	5.05	116.81	108.13
1	A	142	LYS	N-CA-C	-5.03	105.31	111.75
2	B	2140	PHE	CA-C-N	5.03	126.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2140	PHE	C-N-CA	5.03	126.98	120.44
2	B	2098	ILE	N-CA-CB	5.02	116.19	110.72
1	A	145	GLY	CA-C-N	5.02	125.80	120.13
1	A	145	GLY	C-N-CA	5.02	125.80	120.13
1	A	516	THR	CB-CA-C	-5.02	99.19	109.38
2	B	2008	ALA	N-CA-C	-5.02	106.31	114.09
2	B	2286	ASN	N-CA-C	5.01	116.41	110.19

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ALA	Peptide
1	A	436	PHE	Peptide
1	A	547	LEU	Peptide
1	A	583	ARG	Peptide
1	A	693	HIS	Peptide
2	B	1710	GLY	Peptide
2	B	2141	ASN	Peptide
2	B	2319	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4944	0	4834	429	0
2	B	4929	0	4812	407	0
3	C	28	0	25	2	0
4	D	61	0	52	3	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	4	0	6	3	0
7	B	4	0	6	0	0
8	B	1	0	0	0	0
All	All	9973	0	9735	822	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 42.

All (822) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:THR:HG22	1:A:677:THR:HB	1.26	1.17
2:B:1733:VAL:HG22	2:B:1890:TYR:HE2	1.12	1.13
1:A:523:LYS:H	1:A:523:LYS:HD3	1.05	1.13
2:B:2266:GLN:HE21	2:B:2266:GLN:HA	1.01	1.11
2:B:1859:HIS:O	2:B:1862:THR:HG22	1.55	1.05
1:A:271:LEU:HD23	1:A:274:HIS:HB2	1.40	1.04
1:A:53:GLU:HB2	1:A:63:LYS:CB	1.88	1.03
1:A:150:ASP:HB2	1:A:151:PRO:HD2	1.41	1.03
2:B:1711:MET:HG3	2:B:1712:SER:H	1.25	1.02
2:B:2045:GLN:O	2:B:2046:TRP:HB2	1.57	1.02
4:D:1:NAG:H3	4:D:2:NAG:H2	1.43	1.01
1:A:14:TRP:HD1	1:A:231:MET:HE1	1.19	1.00
1:A:53:GLU:CB	1:A:63:LYS:HB2	1.91	1.00
1:A:53:GLU:HB2	1:A:63:LYS:HB2	1.02	1.00
1:A:595:LEU:HD13	1:A:596:PRO:HD2	1.44	0.99
1:A:575:LEU:HD13	1:A:642:ILE:HG22	1.46	0.98
1:A:530:THR:CG2	1:A:677:THR:HB	1.93	0.98
2:B:1870:GLN:HG3	2:B:1871:VAL:H	1.26	0.98
2:B:2141:ASN:HB2	2:B:2142:PRO:CD	1.92	0.98
1:A:127:LYS:HG2	1:A:162:VAL:HG11	1.46	0.97
1:A:575:LEU:CD1	1:A:642:ILE:HG22	1.96	0.95
1:A:76:ILE:HD11	1:A:176:LEU:HD13	1.47	0.95
1:A:495:VAL:HG21	1:A:501:PHE:HB2	1.46	0.94
1:A:52:VAL:CG2	1:A:53:GLU:H	1.80	0.94
2:B:2061:ALA:HB2	2:B:2163:ARG:HG3	1.50	0.93
2:B:1893:GLU:HA	2:B:1893:GLU:OE1	1.69	0.93
2:B:2000:CYS:SG	2:B:2002:ILE:HG12	2.10	0.92
1:A:523:LYS:HD3	1:A:523:LYS:N	1.85	0.91
2:B:2027:MET:HG3	2:B:2032:ILE:HD12	1.51	0.91
2:B:1733:VAL:HG22	2:B:1890:TYR:CE2	2.05	0.91
1:A:52:VAL:CG2	1:A:53:GLU:N	2.32	0.91
1:A:14:TRP:CD1	1:A:231:MET:HE1	2.04	0.91
2:B:2105:TYR:HD2	2:B:2146:ALA:HB2	1.34	0.91
1:A:229:PRO:O	1:A:230:LYS:HB2	1.71	0.90
1:A:62:ALA:H	1:A:63:LYS:HE3	1.36	0.90
1:A:299:LEU:HG	1:A:299:LEU:O	1.71	0.89
1:A:523:LYS:H	1:A:523:LYS:CD	1.83	0.89
1:A:146:PRO:HA	1:A:154:LEU:HD11	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2266:GLN:HA	2:B:2266:GLN:NE2	1.79	0.89
2:B:2266:GLN:HE21	2:B:2266:GLN:CA	1.86	0.89
1:A:14:TRP:O	1:A:15:ASP:HB2	1.72	0.88
1:A:615:HIS:O	1:A:621:VAL:HG12	1.73	0.88
1:A:52:VAL:HG22	1:A:53:GLU:N	1.89	0.88
1:A:52:VAL:HG23	1:A:53:GLU:H	1.38	0.87
2:B:2244:THR:HG23	2:B:2294:VAL:HB	1.54	0.87
1:A:46:TYR:OH	1:A:229:PRO:HA	1.75	0.87
1:A:449:LEU:HD12	1:A:449:LEU:H	1.38	0.86
1:A:457:VAL:HA	1:A:515:VAL:CG1	2.07	0.85
1:A:290:PRO:HG2	2:B:1953:ILE:HG12	1.57	0.85
2:B:1859:HIS:O	2:B:1862:THR:CG2	2.25	0.84
1:A:527:ARG:HE	1:A:555:TYR:HD2	1.26	0.84
1:A:610:ALA:HA	1:A:613:ILE:HD12	1.60	0.84
2:B:2039:ALA:HB2	2:B:2048:PRO:HG3	1.60	0.84
1:A:79:GLU:O	1:A:140:VAL:HG21	1.77	0.84
2:B:2059:ILE:HD13	2:B:2059:ILE:O	1.78	0.83
2:B:1863:LEU:HD22	2:B:1869:ARG:HB3	1.61	0.83
2:B:2023:THR:OG1	2:B:2024:PRO:HD2	1.77	0.83
1:A:147:MET:HE2	2:B:1972:LYS:HB2	1.60	0.82
1:A:417:GLN:HA	1:A:595:LEU:HD11	1.61	0.82
1:A:456:GLU:O	1:A:459:ASP:HB2	1.80	0.82
1:A:61:ILE:HG13	1:A:63:LYS:NZ	1.94	0.82
2:B:2176:MET:HE3	2:B:2177:PRO:HD2	1.61	0.82
1:A:457:VAL:HA	1:A:515:VAL:HG12	1.62	0.82
2:B:1924:TYR:CD2	2:B:1929:LEU:HA	2.15	0.81
1:A:430:ALA:O	1:A:439:ARG:HB3	1.80	0.81
2:B:2006:LEU:HD23	2:B:2010:MET:HB2	1.61	0.81
1:A:85:VAL:HG22	1:A:137:VAL:HG23	1.62	0.81
2:B:1732:LYS:HE3	2:B:1885:GLU:OE2	1.80	0.81
1:A:245:LEU:H	1:A:245:LEU:HD22	1.45	0.80
1:A:234:VAL:O	1:A:235:ASN:HB2	1.82	0.80
2:B:2141:ASN:HB2	2:B:2142:PRO:HD2	1.61	0.80
1:A:271:LEU:HD12	1:A:308:LEU:HB3	1.63	0.80
2:B:1793:GLU:O	2:B:1794:GLU:HB2	1.79	0.80
2:B:2193:SER:O	2:B:2194:SER:HB3	1.82	0.79
1:A:409:SER:O	1:A:410:GLN:HB2	1.81	0.79
1:A:9:ALA:HB3	1:A:90:ASN:HA	1.65	0.79
2:B:2224:ASN:HD22	2:B:2317:ILE:HD12	1.45	0.79
1:A:521:PRO:HG3	1:A:529:LEU:HG	1.65	0.78
1:A:575:LEU:HD13	1:A:642:ILE:CG2	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1709:TYR:OH	2:B:1918:PHE:CD2	2.36	0.78
2:B:2314:VAL:HG13	2:B:2315:HIS:H	1.47	0.78
1:A:575:LEU:HD11	1:A:577:SER:HB2	1.64	0.78
2:B:2046:TRP:HH2	2:B:2058:SER:O	1.64	0.78
2:B:1807:VAL:HG11	2:B:1813:LYS:HB2	1.65	0.78
2:B:1739:THR:CG2	2:B:1740:ASP:H	1.96	0.78
1:A:61:ILE:HG13	1:A:63:LYS:HZ1	1.49	0.77
2:B:1858:CYS:HB3	2:B:1862:THR:HG21	1.65	0.77
2:B:1870:GLN:O	2:B:1871:VAL:HB	1.85	0.76
1:A:1:ALA:O	1:A:2:THR:HB	1.85	0.76
2:B:1918:PHE:HA	2:B:1925:ILE:HD12	1.66	0.76
2:B:2298:ASP:HB3	2:B:2299:PRO:HD3	1.67	0.76
2:B:1739:THR:HG23	2:B:1740:ASP:N	1.99	0.76
1:A:147:MET:HE1	2:B:1972:LYS:NZ	2.01	0.76
2:B:2214:GLY:H	2:B:2217:ASN:HD22	1.33	0.76
1:A:453:LEU:HD23	1:A:513:TRP:CZ3	2.21	0.76
1:A:163:ASP:HB3	1:A:166:LYS:HB3	1.67	0.76
1:A:660:HIS:C	1:A:661:LYS:HD3	2.11	0.76
2:B:2314:VAL:HG13	2:B:2315:HIS:N	1.99	0.76
1:A:555:TYR:HD1	1:A:556:LYS:H	1.34	0.75
2:B:1752:LEU:HD11	2:B:2118:ASN:HA	1.68	0.75
2:B:2048:PRO:HD3	2:B:2062:TRP:CD1	2.20	0.75
1:A:592:GLN:HA	1:A:598:PRO:HG2	1.69	0.75
2:B:1870:GLN:CG	2:B:1871:VAL:H	2.00	0.75
2:B:2025:LEU:HD12	2:B:2166:LEU:HB3	1.68	0.74
1:A:109:SER:O	1:A:110:GLU:HB3	1.85	0.74
2:B:1739:THR:HG23	2:B:1740:ASP:H	1.53	0.74
1:A:61:ILE:CG1	1:A:63:LYS:HZ1	2.00	0.74
1:A:77:GLN:HG3	1:A:177:LEU:HB2	1.70	0.74
2:B:1870:GLN:HG3	2:B:1871:VAL:N	1.99	0.73
1:A:198:LEU:H	1:A:235:ASN:ND2	1.86	0.73
2:B:2087:GLN:HA	2:B:2129:ASN:HD21	1.53	0.73
1:A:100:ALA:HB2	1:A:138:TRP:CZ2	2.24	0.73
1:A:527:ARG:O	1:A:528:CYS:HB2	1.87	0.73
2:B:2156:TYR:HD1	2:B:2156:TYR:N	1.87	0.73
2:B:2256:TYR:H	2:B:2314:VAL:HG12	1.53	0.73
1:A:150:ASP:HB2	1:A:151:PRO:CD	2.19	0.72
2:B:1764:ARG:HD3	2:B:1869:ARG:HB2	1.71	0.72
2:B:2256:TYR:H	2:B:2314:VAL:CG1	2.02	0.72
1:A:453:LEU:HD23	1:A:513:TRP:HZ3	1.53	0.72
2:B:1733:VAL:CG2	2:B:1890:TYR:HE2	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1735:PHE:CE2	2:B:1851:LEU:HB3	2.25	0.72
2:B:2156:TYR:HD2	2:B:2160:SER:N	1.87	0.72
1:A:426:VAL:HG13	1:A:547:LEU:HD22	1.70	0.71
1:A:63:LYS:O	1:A:63:LYS:HG2	1.89	0.71
1:A:209:HIS:HE1	1:A:229:PRO:HG3	1.54	0.71
2:B:2045:GLN:NE2	2:B:2050:LEU:HD11	2.05	0.71
2:B:2064:THR:HG21	2:B:2066:GLU:HG2	1.71	0.71
2:B:2108:ASP:CG	2:B:2109:GLY:H	1.97	0.71
1:A:16:TYR:N	1:A:16:TYR:CD1	2.58	0.71
1:A:471:ARG:NH1	1:A:471:ARG:HB2	2.05	0.71
1:A:471:ARG:HB2	1:A:471:ARG:CZ	2.20	0.71
2:B:1976:TYR:CZ	2:B:1984:GLU:HG2	2.26	0.70
1:A:150:ASP:CB	1:A:151:PRO:HD2	2.13	0.70
1:A:682:MET:CG	1:A:682:MET:O	2.36	0.70
2:B:1830:PHE:HE1	2:B:1970:GLU:OE2	1.75	0.70
1:A:460:THR:HG23	1:A:514:THR:HG23	1.74	0.70
2:B:1739:THR:CG2	2:B:1740:ASP:N	2.54	0.70
2:B:1941:ARG:HD2	2:B:1943:TYR:CZ	2.25	0.70
1:A:331:GLU:H	1:A:331:GLU:CD	1.99	0.70
1:A:419:ILE:HD13	1:A:419:ILE:H	1.57	0.70
2:B:2087:GLN:HA	2:B:2129:ASN:ND2	2.06	0.70
2:B:1781:ARG:HB3	2:B:1889:TRP:CZ3	2.26	0.69
2:B:1826:THR:N	2:B:1829:GLU:HG3	2.08	0.69
2:B:1734:VAL:HG12	2:B:1735:PHE:N	2.06	0.69
1:A:383:VAL:HG22	1:A:462:LEU:HB3	1.75	0.69
1:A:16:TYR:N	1:A:16:TYR:HD1	1.91	0.69
1:A:165:VAL:HG13	1:A:262:THR:OG1	1.92	0.68
2:B:2002:ILE:HG13	2:B:2005:HIS:HB2	1.75	0.68
2:B:2322:GLU:HG3	2:B:2323:VAL:H	1.57	0.68
1:A:50:LEU:HB3	1:A:171:GLY:O	1.93	0.68
1:A:199:PHE:HB3	1:A:320:MET:HE1	1.74	0.68
1:A:127:LYS:HG2	1:A:162:VAL:CG1	2.22	0.68
1:A:310:CYS:SG	1:A:312:ILE:HG12	2.34	0.68
2:B:2193:SER:HB3	2:B:2229:TRP:CE2	2.29	0.68
2:B:2195:TYR:HA	2:B:2221:PRO:HA	1.76	0.68
1:A:241:SER:O	1:A:242:LEU:HB2	1.92	0.68
1:A:269:ILE:N	1:A:269:ILE:HD12	2.08	0.68
2:B:1953:ILE:HD12	2:B:1979:TYR:CE1	2.29	0.68
1:A:46:TYR:O	1:A:47:LYS:HG3	1.94	0.67
1:A:55:THR:HG22	1:A:62:ALA:CB	2.23	0.67
2:B:2087:GLN:HB3	2:B:2163:ARG:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1829:GLU:OE2	2:B:1833:LYS:HE2	1.94	0.67
1:A:11:GLU:HA	1:A:49:THR:HA	1.75	0.67
2:B:2286:ASN:ND2	2:B:2286:ASN:H	1.92	0.67
2:B:2050:LEU:O	2:B:2061:ALA:HA	1.94	0.67
2:B:2276:GLN:HG3	2:B:2298:ASP:OD2	1.94	0.67
2:B:2141:ASN:CB	2:B:2142:PRO:HD2	2.25	0.67
1:A:45:VAL:C	1:A:47:LYS:HZ1	2.03	0.67
1:A:184:LEU:HD13	1:A:190:GLN:HE21	1.60	0.66
2:B:1709:TYR:HH	2:B:1918:PHE:HD2	1.38	0.66
1:A:306:PHE:HE2	1:A:326:VAL:CG1	2.08	0.66
2:B:2182:SER:C	2:B:2184:ALA:H	2.02	0.66
1:A:642:ILE:HD12	1:A:673:PHE:CD1	2.30	0.66
2:B:2080:ILE:HD12	2:B:2082:HIS:CE1	2.30	0.66
2:B:2105:TYR:CD2	2:B:2146:ALA:HB2	2.23	0.66
2:B:2147:ARG:HD3	2:B:2148:TYR:CE1	2.31	0.66
1:A:486:LEU:HD23	1:A:487:TYR:CE1	2.31	0.66
1:A:489:ARG:HG3	1:A:489:ARG:HH11	1.61	0.66
1:A:278:VAL:O	1:A:280:ASN:N	2.28	0.66
2:B:2102:ILE:C	2:B:2102:ILE:HD12	2.20	0.66
1:A:636:TYR:CD1	1:A:679:PHE:HD1	2.14	0.66
1:A:11:GLU:HB3	1:A:49:THR:HB	1.75	0.65
1:A:61:ILE:O	1:A:62:ALA:HB2	1.96	0.65
2:B:1708:ASP:C	2:B:1709:TYR:CD1	2.75	0.65
1:A:408:LYS:HB3	1:A:622:PHE:CE1	2.31	0.65
1:A:641:SER:HB2	1:A:649:LEU:HD12	1.78	0.65
2:B:2118:ASN:O	2:B:2120:THR:HG22	1.96	0.65
1:A:691:GLY:HA3	1:A:703:THR:HG22	1.78	0.65
2:B:2027:MET:O	2:B:2052:ARG:HB3	1.96	0.65
1:A:128:VAL:HG11	1:A:132:GLY:O	1.97	0.65
2:B:2046:TRP:CH2	2:B:2058:SER:O	2.47	0.65
2:B:2141:ASN:HB2	2:B:2142:PRO:HD3	1.75	0.65
2:B:2314:VAL:CG1	2:B:2315:HIS:H	2.09	0.65
2:B:2080:ILE:HG22	2:B:2145:ILE:HD13	1.79	0.65
2:B:2322:GLU:CG	2:B:2323:VAL:N	2.60	0.65
2:B:1921:ILE:CD1	2:B:2010:MET:O	2.45	0.64
1:A:155:THR:HG22	1:A:293:PHE:HB3	1.79	0.64
2:B:1921:ILE:HD11	2:B:2010:MET:O	1.97	0.64
2:B:2156:TYR:N	2:B:2156:TYR:CD1	2.60	0.64
2:B:1698:TYR:CD2	2:B:1763:ILE:HG23	2.32	0.64
1:A:400:LEU:HB3	1:A:402:PRO:HD3	1.80	0.64
2:B:1709:TYR:CD1	2:B:1709:TYR:N	2.66	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2276:GLN:HB2	2:B:2281:LYS:HB2	1.78	0.64
1:A:245:LEU:HD22	1:A:245:LEU:N	2.11	0.63
2:B:2006:LEU:C	2:B:2008:ALA:H	2.04	0.63
2:B:1848:HIS:HD2	2:B:1884:ASP:H	1.46	0.63
1:A:460:THR:HG23	1:A:514:THR:HA	1.78	0.63
1:A:483:VAL:HG13	1:A:513:TRP:CD1	2.34	0.63
2:B:1826:THR:H	2:B:1829:GLU:HG3	1.62	0.63
1:A:68:TRP:H	1:A:68:TRP:CD1	2.14	0.63
1:A:137:VAL:CG1	1:A:137:VAL:O	2.47	0.63
2:B:2322:GLU:CG	2:B:2323:VAL:H	2.11	0.63
1:A:169:ASN:OD1	1:A:203:ASP:HB3	1.99	0.62
2:B:1946:SER:HB2	2:B:1978:LEU:HB3	1.80	0.62
2:B:2186:SER:HB3	2:B:2189:GLN:OE1	2.00	0.62
2:B:1914:GLU:CD	2:B:1915:ASN:N	2.58	0.62
1:A:67:PRO:HB3	1:A:243:PRO:HG2	1.82	0.62
1:A:419:ILE:HG22	1:A:594:PHE:CB	2.29	0.62
2:B:1807:VAL:CG1	2:B:1813:LYS:HB2	2.29	0.62
2:B:1924:TYR:CE2	2:B:1930:PRO:HD3	2.33	0.62
1:A:662:MET:HB2	2:B:1968:LYS:NZ	2.15	0.62
1:A:437:LYS:O	1:A:438:THR:OG1	2.15	0.62
1:A:160:SER:HB3	1:A:167:ASP:HB3	1.82	0.62
1:A:582:ASN:O	1:A:587:LEU:HD13	2.00	0.62
1:A:643:GLY:HA2	1:A:645:GLN:HE22	1.63	0.62
1:A:483:VAL:HG13	1:A:513:TRP:HD1	1.64	0.62
2:B:2117:GLY:O	2:B:2118:ASN:O	2.17	0.61
1:A:542:ASP:O	1:A:547:LEU:HB2	1.99	0.61
2:B:2298:ASP:CB	2:B:2299:PRO:CD	2.78	0.61
1:A:169:ASN:HD21	1:A:262:THR:HB	1.65	0.61
1:A:661:LYS:O	1:A:661:LYS:HG2	2.01	0.61
1:A:682:MET:O	1:A:682:MET:HG2	2.01	0.61
2:B:1790:ILE:HG23	2:B:1790:ILE:O	2.01	0.61
1:A:233:THR:OG1	1:A:234:VAL:N	2.31	0.61
2:B:2250:SER:C	2:B:2252:LEU:H	2.07	0.61
2:B:1739:THR:HG21	2:B:1745:GLN:HB2	1.81	0.61
2:B:1781:ARG:HG3	2:B:1889:TRP:HE3	1.66	0.60
2:B:2298:ASP:CB	2:B:2299:PRO:HD3	2.30	0.60
1:A:137:VAL:O	1:A:137:VAL:HG13	2.00	0.60
2:B:2304:ARG:HD2	2:B:2305:TYR:CE2	2.35	0.60
1:A:141:LEU:H	1:A:141:LEU:HD12	1.67	0.60
2:B:1732:LYS:HG2	2:B:1849:SER:O	2.02	0.60
1:A:460:THR:HG21	1:A:512:LYS:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1767:VAL:O	2:B:1819:VAL:HB	2.02	0.60
1:A:575:LEU:HG	1:A:575:LEU:O	2.00	0.60
1:A:241:SER:O	1:A:242:LEU:CB	2.49	0.60
2:B:2060:ASN:OD1	2:B:2163:ARG:HD3	2.01	0.60
1:A:433:ASP:OD2	1:A:435:THR:HG23	2.02	0.60
2:B:2046:TRP:CZ3	2:B:2059:ILE:HA	2.36	0.59
2:B:1711:MET:HG3	2:B:1712:SER:N	2.07	0.59
2:B:2314:VAL:CG1	2:B:2315:HIS:N	2.65	0.59
1:A:636:TYR:HD1	1:A:679:PHE:HD1	1.50	0.59
1:A:207:SER:HB3	1:A:209:HIS:H	1.66	0.59
1:A:146:PRO:CA	1:A:154:LEU:HD11	2.31	0.59
2:B:1951:GLU:O	2:B:1953:ILE:N	2.31	0.59
1:A:82:ASP:O	1:A:140:VAL:HG22	2.03	0.59
1:A:289:SER:CB	1:A:290:PRO:HD2	2.33	0.59
1:A:529:LEU:HD12	1:A:553:ILE:O	2.03	0.59
1:A:624:SER:O	1:A:625:LEU:HB3	2.01	0.59
2:B:1699:PHE:HD2	2:B:1739:THR:O	1.85	0.59
1:A:605:ASP:OD2	1:A:608:PHE:HB3	2.03	0.59
2:B:2048:PRO:O	2:B:2049:LYS:CB	2.50	0.59
2:B:1977:ASN:HD22	2:B:1977:ASN:H	1.50	0.59
1:A:587:LEU:HD23	1:A:588:THR:HG22	1.84	0.58
2:B:1941:ARG:HD2	2:B:1943:TYR:CE1	2.38	0.58
2:B:2291:THR:HG22	2:B:2291:THR:O	2.03	0.58
1:A:147:MET:HE1	2:B:1972:LYS:HZ1	1.67	0.58
1:A:157:SER:HA	1:A:176:LEU:HB3	1.85	0.58
2:B:1893:GLU:OE1	2:B:1893:GLU:CA	2.49	0.58
2:B:2147:ARG:HD3	2:B:2148:TYR:HE1	1.68	0.58
2:B:1732:LYS:CE	2:B:1885:GLU:OE2	2.51	0.58
1:A:7:LEU:HD21	1:A:51:PHE:CD1	2.37	0.58
1:A:405:ARG:HG3	1:A:406:SER:N	2.18	0.58
2:B:2076:LEU:O	2:B:2077:ALA:CB	2.51	0.58
1:A:80:VAL:O	1:A:81:TYR:CD2	2.57	0.58
2:B:1881:THR:HG23	2:B:1952:ASN:HD21	1.68	0.58
2:B:1826:THR:C	2:B:1828:ASP:H	2.11	0.58
1:A:118:THR:HB	1:A:122:GLU:HB2	1.86	0.58
1:A:410:GLN:CG	1:A:418:ARG:HH12	2.17	0.58
1:A:693:HIS:O	1:A:693:HIS:HD2	1.86	0.58
2:B:2048:PRO:O	2:B:2049:LYS:HB3	2.02	0.58
2:B:2076:LEU:O	2:B:2077:ALA:HB2	2.02	0.58
2:B:2108:ASP:CG	2:B:2109:GLY:N	2.59	0.58
1:A:245:LEU:HB3	1:A:324:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HA	1:A:309:PHE:O	2.03	0.58
1:A:62:ALA:N	1:A:63:LYS:HE3	2.11	0.58
2:B:2045:GLN:HE21	2:B:2050:LEU:HD11	1.66	0.57
1:A:477:PRO:HG3	1:A:513:TRP:CE2	2.39	0.57
2:B:1934:MET:HE2	2:B:2016:VAL:HG12	1.87	0.57
2:B:2000:CYS:SG	2:B:2002:ILE:CG1	2.88	0.57
2:B:2192:ALA:HB2	2:B:2230:LEU:HD12	1.85	0.57
1:A:4:ARG:HD3	1:A:6:TYR:HE1	1.70	0.57
1:A:48:LYS:HA	1:A:208:TRP:HZ2	1.69	0.57
1:A:595:LEU:HD13	1:A:596:PRO:CD	2.28	0.57
1:A:181:GLU:OE1	1:A:181:GLU:N	2.38	0.57
2:B:2049:LYS:C	2:B:2051:ALA:H	2.11	0.57
1:A:623:ASP:HB3	1:A:705:LEU:HD11	1.87	0.57
1:A:660:HIS:O	1:A:661:LYS:HD3	2.04	0.57
1:A:61:ILE:O	1:A:62:ALA:CB	2.52	0.57
1:A:278:VAL:O	1:A:279:ARG:C	2.47	0.57
2:B:2182:SER:C	2:B:2184:ALA:N	2.63	0.57
1:A:105:TYR:CE1	1:A:110:GLU:HB2	2.40	0.56
1:A:680:MET:HB3	1:A:682:MET:HE3	1.86	0.56
2:B:2028:ALA:HB2	2:B:2165:GLU:OE2	2.05	0.56
2:B:2250:SER:HB3	2:B:2252:LEU:HB2	1.87	0.56
2:B:1709:TYR:OH	2:B:1918:PHE:HD2	1.84	0.56
1:A:115:ASP:HB3	1:A:117:GLN:OE1	2.06	0.56
1:A:116:ASP:O	1:A:117:GLN:HB2	2.03	0.56
1:A:163:ASP:O	1:A:165:VAL:N	2.38	0.56
1:A:252:SER:HA	1:A:299:LEU:HA	1.88	0.56
1:A:401:ALA:CB	1:A:408:LYS:HE3	2.34	0.56
2:B:1733:VAL:HB	2:B:1851:LEU:HD11	1.86	0.56
2:B:1934:MET:HE2	2:B:2016:VAL:CG1	2.35	0.56
2:B:2023:THR:OG1	2:B:2024:PRO:CD	2.52	0.56
2:B:2250:SER:C	2:B:2252:LEU:N	2.62	0.56
1:A:290:PRO:HB3	2:B:2002:ILE:HG21	1.86	0.56
1:A:428:PHE:CZ	1:A:475:ILE:HG23	2.40	0.56
1:A:578:VAL:HG12	1:A:644:ALA:HA	1.87	0.56
1:A:113:GLU:HB2	1:A:126:ASP:HB3	1.88	0.56
2:B:2286:ASN:H	2:B:2286:ASN:HD22	1.51	0.56
1:A:156:TYR:O	1:A:157:SER:HB3	2.05	0.56
1:A:50:LEU:HD22	1:A:71:LEU:HB2	1.88	0.56
1:A:687:LEU:H	2:B:1803:ARG:HG3	1.71	0.56
1:A:693:HIS:O	1:A:693:HIS:CD2	2.59	0.55
1:A:71:LEU:HD21	1:A:202:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1883:PHE:HB2	2:B:1918:PHE:HB2	1.87	0.55
1:A:416:PRO:O	1:A:596:PRO:HG2	2.06	0.55
1:A:484:ARG:HD2	1:A:489:ARG:HG2	1.88	0.55
1:A:697:PHE:O	1:A:699:ASN:N	2.40	0.55
2:B:2151:LEU:C	2:B:2151:LEU:HD12	2.32	0.55
2:B:2116:ARG:HG3	2:B:2120:THR:CG2	2.37	0.55
1:A:80:VAL:HG23	1:A:181:GLU:OE1	2.07	0.55
2:B:1781:ARG:HG3	2:B:1889:TRP:CE3	2.40	0.55
1:A:60:ASN:HD22	1:A:61:ILE:HG22	1.72	0.55
1:A:62:ALA:H	1:A:63:LYS:CE	2.16	0.55
2:B:1892:THR:O	2:B:1893:GLU:HB2	2.07	0.55
2:B:2281:LYS:HE2	2:B:2281:LYS:HA	1.88	0.55
1:A:446:SER:HA	1:A:618:ASN:HD22	1.73	0.55
1:A:158:TYR:CZ	1:A:174:GLY:HA3	2.42	0.54
1:A:575:LEU:CD1	1:A:642:ILE:CG2	2.76	0.54
2:B:1953:ILE:HD12	2:B:1979:TYR:HE1	1.69	0.54
1:A:309:PHE:HB3	1:A:321:GLU:HB3	1.90	0.54
1:A:480:ILE:HG22	1:A:481:THR:H	1.71	0.54
2:B:2179:GLY:HA2	2:B:2182:SER:HB2	1.89	0.54
2:B:1782:PRO:O	2:B:1783:TYR:CD1	2.60	0.54
2:B:1914:GLU:CD	2:B:1915:ASN:H	2.15	0.54
2:B:1953:ILE:CD1	2:B:1979:TYR:CE1	2.89	0.54
1:A:145:GLY:O	2:B:1972:LYS:HD2	2.08	0.54
2:B:1888:SER:C	2:B:1890:TYR:H	2.15	0.54
1:A:463:ILE:HG21	1:A:475:ILE:HD12	1.89	0.54
1:A:80:VAL:O	1:A:81:TYR:CG	2.61	0.54
1:A:108:ALA:HA	1:A:125:ASP:OD1	2.08	0.54
2:B:1785:PHE:HB2	2:B:1815:TYR:CE1	2.42	0.54
2:B:1997:ARG:CZ	2:B:2011:SER:HB2	2.36	0.54
1:A:5:TYR:CE2	1:A:76:ILE:HB	2.43	0.54
1:A:529:LEU:HA	1:A:677:THR:HG21	1.89	0.54
1:A:555:TYR:CD1	1:A:556:LYS:N	2.73	0.54
2:B:1941:ARG:HD2	2:B:1943:TYR:OH	2.08	0.54
2:B:2263:SER:HA	2:B:2273:LEU:HA	1.90	0.54
2:B:1785:PHE:CB	2:B:1815:TYR:CE1	2.91	0.54
2:B:2296:SER:O	2:B:2297:LEU:HD23	2.08	0.54
1:A:662:MET:HB2	2:B:1968:LYS:HZ2	1.73	0.54
2:B:2304:ARG:HD2	2:B:2305:TYR:CD2	2.42	0.54
1:A:68:TRP:O	1:A:70:GLY:N	2.38	0.53
2:B:2034:ASP:OD2	2:B:2049:LYS:HE3	2.08	0.53
2:B:2207:LYS:O	2:B:2212:LEU:HD23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLN:C	1:A:418:ARG:HG2	2.33	0.53
1:A:419:ILE:HG22	1:A:594:PHE:HB2	1.90	0.53
1:A:152:LEU:HG	1:A:180:ARG:HH12	1.74	0.53
1:A:587:LEU:HG	1:A:588:THR:N	2.23	0.53
1:A:7:LEU:HD21	1:A:51:PHE:HD1	1.74	0.53
2:B:2046:TRP:HD1	2:B:2063:SER:HB3	1.74	0.53
2:B:2102:ILE:CG2	2:B:2123:LEU:HD21	2.38	0.53
1:A:183:SER:H	1:A:187:GLU:HB3	1.72	0.53
1:A:457:VAL:HA	1:A:515:VAL:HG11	1.89	0.53
2:B:1924:TYR:HD2	2:B:1929:LEU:HA	1.69	0.53
2:B:2038:THR:O	2:B:2071:ILE:HG13	2.08	0.53
2:B:2248:VAL:HG22	2:B:2318:ALA:HB1	1.91	0.53
2:B:2141:ASN:ND2	2:B:2141:ASN:H	2.07	0.53
1:A:186:LYS:O	1:A:187:GLU:CB	2.57	0.53
1:A:477:PRO:HG3	1:A:513:TRP:CD2	2.44	0.53
2:B:2046:TRP:HZ3	2:B:2059:ILE:HA	1.73	0.53
1:A:94:HIS:NE2	1:A:166:LYS:HG2	2.24	0.53
1:A:267:HIS:CE1	1:A:320:MET:HE3	2.44	0.53
1:A:405:ARG:CG	1:A:406:SER:N	2.72	0.53
1:A:6:TYR:CD2	1:A:56:ASP:O	2.62	0.53
1:A:308:LEU:HD23	1:A:322:ALA:O	2.09	0.53
2:B:2261:LEU:O	2:B:2309:HIS:HB2	2.08	0.53
2:B:2212:LEU:HG	2:B:2217:ASN:HB2	1.90	0.52
1:A:622:PHE:O	1:A:624:SER:N	2.42	0.52
2:B:1709:TYR:CD2	2:B:1925:ILE:HG22	2.44	0.52
2:B:2089:ALA:O	2:B:2096:LEU:HB3	2.10	0.52
2:B:2117:GLY:O	2:B:2118:ASN:C	2.53	0.52
2:B:2156:TYR:HD1	2:B:2156:TYR:H	1.56	0.52
2:B:2178:LEU:HD12	2:B:2323:VAL:HG12	1.91	0.52
1:A:118:THR:HB	1:A:122:GLU:CB	2.38	0.52
1:A:586:TYR:O	1:A:587:LEU:C	2.52	0.52
2:B:1767:VAL:HG23	2:B:1768:GLU:N	2.25	0.52
2:B:1976:TYR:CE1	2:B:1984:GLU:HG2	2.44	0.52
1:A:53:GLU:CD	1:A:74:PRO:HB3	2.35	0.52
2:B:1789:LEU:HD22	2:B:1823:MET:HB3	1.91	0.52
2:B:1888:SER:C	2:B:1890:TYR:N	2.67	0.52
1:A:312:ILE:HD11	1:A:315:HIS:CE1	2.44	0.52
3:C:2:NAG:H5	3:C:2:NAG:N2	2.25	0.52
1:A:53:GLU:OE2	1:A:74:PRO:HB3	2.09	0.52
2:B:2248:VAL:CG2	2:B:2318:ALA:HB1	2.40	0.52
1:A:188:LYS:NZ	1:A:188:LYS:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLN:O	1:A:469:ALA:HB2	2.08	0.52
1:A:79:GLU:O	1:A:140:VAL:CG2	2.55	0.51
1:A:631:LEU:O	1:A:632:HIS:HB2	2.10	0.51
1:A:234:VAL:O	1:A:235:ASN:CB	2.56	0.51
1:A:555:TYR:HD1	1:A:556:LYS:N	2.06	0.51
1:A:667:THR:HG21	1:A:693:HIS:CE1	2.44	0.51
1:A:198:LEU:H	1:A:235:ASN:HD21	1.57	0.51
1:A:541:ARG:O	1:A:545:SER:N	2.43	0.51
2:B:2193:SER:O	2:B:2194:SER:CB	2.53	0.51
2:B:2265:SER:OG	2:B:2266:GLN:N	2.42	0.51
1:A:307:LEU:HG	1:A:309:PHE:CD1	2.45	0.51
1:A:401:ALA:O	1:A:402:PRO:O	2.29	0.51
1:A:433:ASP:N	1:A:433:ASP:OD1	2.40	0.51
1:A:538:ASN:O	1:A:540:GLU:N	2.44	0.51
2:B:1700:ILE:HD11	2:B:1761:PRO:HD2	1.91	0.51
2:B:1767:VAL:CG2	2:B:1768:GLU:N	2.74	0.51
2:B:2234:PHE:HZ	2:B:2323:VAL:HG11	1.75	0.51
1:A:14:TRP:CG	1:A:15:ASP:N	2.79	0.51
2:B:1781:ARG:HB3	2:B:1889:TRP:HZ3	1.74	0.51
1:A:622:PHE:O	1:A:623:ASP:C	2.53	0.51
2:B:1734:VAL:HG12	2:B:1735:PHE:H	1.73	0.51
2:B:2207:LYS:HD2	2:B:2216:SER:O	2.11	0.51
2:B:1878:LEU:HA	2:B:1922:ASN:OD1	2.10	0.51
2:B:2298:ASP:HB3	2:B:2299:PRO:CD	2.37	0.51
2:B:1826:THR:C	2:B:1828:ASP:N	2.69	0.51
1:A:45:VAL:C	1:A:47:LYS:NZ	2.68	0.51
1:A:56:ASP:OD2	1:A:59:PHE:C	2.54	0.51
2:B:2012:THR:C	2:B:2013:LEU:HD12	2.36	0.51
1:A:157:SER:HB2	1:A:174:GLY:O	2.10	0.50
1:A:428:PHE:CE1	1:A:475:ILE:HG23	2.46	0.50
2:B:2192:ALA:C	2:B:2194:SER:H	2.19	0.50
1:A:209:HIS:HE1	1:A:229:PRO:CG	2.22	0.50
1:A:472:PRO:HB3	1:A:502:PRO:HB2	1.92	0.50
1:A:582:ASN:OD1	1:A:609:GLN:NE2	2.44	0.50
1:A:596:PRO:O	1:A:597:ASN:C	2.53	0.50
2:B:2129:ASN:OD1	2:B:2129:ASN:N	2.44	0.50
1:A:635:ALA:HB3	1:A:637:TRP:HE1	1.76	0.50
1:A:534:SER:OG	1:A:535:SER:N	2.43	0.50
1:A:588:THR:O	1:A:591:ILE:HG22	2.10	0.50
1:A:642:ILE:HD12	1:A:673:PHE:HD1	1.76	0.50
2:B:2116:ARG:HB2	2:B:2123:LEU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:O	1:A:148:ALA:C	2.55	0.50
1:A:163:ASP:HA	2:B:2007:HIS:HE1	1.76	0.50
2:B:2157:SER:OG	2:B:2158:ILE:N	2.45	0.50
1:A:5:TYR:HE2	1:A:76:ILE:HB	1.77	0.50
1:A:48:LYS:HZ1	1:A:231:MET:CE	2.24	0.50
1:A:430:ALA:HB2	1:A:451:PRO:HG3	1.93	0.50
1:A:643:GLY:O	1:A:645:GLN:CD	2.54	0.50
1:A:146:PRO:HB3	1:A:154:LEU:HG	1.94	0.50
1:A:578:VAL:HG12	1:A:645:GLN:H	1.77	0.50
2:B:2099:SER:HB3	2:B:2155:HIS:C	2.36	0.50
1:A:237:TYR:CD2	1:A:242:LEU:HG	2.46	0.50
1:A:480:ILE:HD11	1:A:551:LEU:HD21	1.93	0.50
1:A:540:GLU:CD	1:A:540:GLU:H	2.20	0.50
2:B:1955:SER:HB3	2:B:1975:LEU:HD21	1.93	0.50
2:B:2077:ALA:H	2:B:2147:ARG:HG3	1.76	0.50
2:B:2330:ASP:O	2:B:2331:LEU:HB2	2.11	0.50
1:A:410:GLN:HG2	1:A:418:ARG:HH12	1.76	0.50
7:A:3333:EDO:H22	2:B:1977:ASN:ND2	2.27	0.50
2:B:1764:ARG:HH11	2:B:1764:ARG:HG2	1.77	0.50
1:A:271:LEU:CD1	1:A:308:LEU:HB3	2.38	0.49
1:A:291:ILE:HG22	2:B:1955:SER:CB	2.42	0.49
1:A:696:ASP:OD1	1:A:696:ASP:N	2.42	0.49
2:B:1709:TYR:HD2	2:B:1924:TYR:HA	1.77	0.49
2:B:2063:SER:HB2	2:B:2161:THR:HG23	1.94	0.49
2:B:2209:ARG:O	2:B:2211:HIS:N	2.45	0.49
1:A:443:GLN:OE1	1:A:443:GLN:HA	2.12	0.49
1:A:647:ASP:O	1:A:672:PRO:HD3	2.11	0.49
1:A:466:LYS:HE2	1:A:468:GLN:HG2	1.94	0.49
1:A:504:LEU:HD23	1:A:505:PRO:HD2	1.93	0.49
2:B:1764:ARG:HD3	2:B:1869:ARG:CB	2.40	0.49
2:B:1919:HIS:H	2:B:1925:ILE:HD12	1.77	0.49
2:B:2080:ILE:CG2	2:B:2145:ILE:HD13	2.41	0.49
2:B:2242:GLY:HA2	2:B:2297:LEU:HG	1.93	0.49
1:A:636:TYR:CD1	1:A:679:PHE:CD1	2.98	0.49
2:B:1759:LEU:HD13	2:B:1922:ASN:HD22	1.78	0.49
2:B:1993:ALA:HA	2:B:2016:VAL:HG23	1.93	0.49
1:A:63:LYS:O	1:A:63:LYS:CG	2.54	0.49
1:A:128:VAL:CG1	1:A:132:GLY:O	2.59	0.49
2:B:1744:THR:HG23	2:B:1745:GLN:H	1.77	0.49
2:B:1865:PRO:O	2:B:1867:HIS:N	2.36	0.49
2:B:2101:PHE:CE2	2:B:2151:LEU:HD22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2303:THR:OG1	2:B:2304:ARG:N	2.45	0.49
1:A:199:PHE:CE2	1:A:269:ILE:HG12	2.48	0.49
1:A:266:VAL:HG22	1:A:267:HIS:H	1.77	0.49
1:A:396:ALA:HB2	1:A:621:VAL:HG23	1.92	0.49
2:B:2275:PHE:CE1	2:B:2280:VAL:HG22	2.48	0.49
1:A:245:LEU:N	1:A:245:LEU:CD2	2.76	0.49
1:A:702:MET:O	1:A:702:MET:HG3	2.13	0.49
2:B:2053:LEU:HA	2:B:2163:ARG:HB3	1.95	0.49
1:A:449:LEU:H	1:A:449:LEU:CD1	2.16	0.49
2:B:1756:LEU:O	2:B:1922:ASN:HB3	2.13	0.49
2:B:2180:MET:O	2:B:2209:ARG:NH1	2.43	0.49
2:B:2224:ASN:ND2	2:B:2317:ILE:HD12	2.23	0.49
1:A:48:LYS:NZ	1:A:231:MET:HE2	2.28	0.48
2:B:1881:THR:HG22	2:B:1882:ILE:O	2.13	0.48
1:A:466:LYS:HB2	1:A:508:ILE:HG22	1.94	0.48
2:B:1739:THR:CG2	2:B:1745:GLN:HB2	2.42	0.48
2:B:1826:THR:O	2:B:1828:ASP:N	2.47	0.48
1:A:267:HIS:HA	1:A:312:ILE:HD13	1.93	0.48
1:A:403:ASP:C	1:A:405:ARG:H	2.20	0.48
1:A:461:LEU:HB2	1:A:513:TRP:HB2	1.95	0.48
1:A:489:ARG:O	1:A:490:ARG:C	2.55	0.48
1:A:6:TYR:HD2	1:A:56:ASP:O	1.95	0.48
1:A:453:LEU:CD1	1:A:453:LEU:N	2.76	0.48
1:A:652:PHE:O	1:A:653:PHE:HB2	2.12	0.48
2:B:1781:ARG:HB3	2:B:1782:PRO:HD2	1.94	0.48
2:B:1879:PHE:CZ	2:B:1881:THR:OG1	2.66	0.48
2:B:1919:HIS:O	2:B:2009:GLY:O	2.31	0.48
1:A:48:LYS:HD3	1:A:170:SER:O	2.14	0.48
1:A:272:GLU:C	1:A:274:HIS:H	2.21	0.48
1:A:485:PRO:HB3	1:A:509:PHE:CZ	2.48	0.48
1:A:588:THR:O	1:A:591:ILE:CG2	2.61	0.48
2:B:1863:LEU:HD23	2:B:1870:GLN:H	1.78	0.48
1:A:48:LYS:NZ	1:A:231:MET:CE	2.77	0.48
1:A:120:GLN:C	1:A:122:GLU:H	2.19	0.48
2:B:2286:ASN:HA	2:B:2293:VAL:HG11	1.96	0.48
1:A:543:LEU:HD23	1:A:544:ALA:N	2.28	0.48
2:B:2025:LEU:HD11	2:B:2168:GLY:HA3	1.95	0.48
2:B:2141:ASN:HB3	4:D:1:NAG:N2	2.29	0.48
1:A:68:TRP:C	1:A:70:GLY:N	2.71	0.48
1:A:271:LEU:HD23	1:A:274:HIS:CB	2.29	0.48
1:A:535:SER:HB3	1:A:542:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ASP:O	1:A:713:LYS:C	2.57	0.48
2:B:1934:MET:O	2:B:2016:VAL:HA	2.13	0.48
1:A:51:PHE:HB2	1:A:73:GLY:HA3	1.96	0.48
1:A:120:GLN:C	1:A:122:GLU:N	2.69	0.48
2:B:1825:PRO:HD3	2:B:1833:LYS:HB2	1.96	0.48
2:B:1934:MET:HE3	2:B:1940:ILE:CD1	2.44	0.48
2:B:1921:ILE:HD12	2:B:2010:MET:O	2.14	0.47
1:A:238:VAL:O	1:A:240:ARG:N	2.46	0.47
2:B:2006:LEU:HB3	2:B:2007:HIS:HD2	1.79	0.47
2:B:2098:ILE:HD13	2:B:2153:PRO:HB3	1.96	0.47
2:B:2214:GLY:N	2:B:2217:ASN:HD22	2.09	0.47
2:B:1912:PHE:O	2:B:1913:LYS:HB2	2.14	0.47
2:B:2162:LEU:HG	2:B:2164:MET:HG2	1.96	0.47
1:A:71:LEU:HD12	1:A:71:LEU:H	1.79	0.47
1:A:453:LEU:N	1:A:453:LEU:HD12	2.29	0.47
2:B:1803:ARG:O	2:B:1804:LYS:HB2	2.14	0.47
2:B:1892:THR:O	2:B:1893:GLU:CB	2.62	0.47
2:B:2118:ASN:O	2:B:2119:SER:C	2.57	0.47
2:B:1698:TYR:CE2	2:B:1763:ILE:HG23	2.49	0.47
2:B:2087:GLN:CA	2:B:2129:ASN:HD21	2.26	0.47
2:B:2102:ILE:C	2:B:2102:ILE:CD1	2.87	0.47
1:A:581:GLU:HB2	1:A:612:ASN:O	2.14	0.47
1:A:645:GLN:HA	1:A:645:GLN:HE21	1.80	0.47
7:A:3333:EDO:H22	2:B:1977:ASN:HD21	1.78	0.47
2:B:1758:LEU:HD12	2:B:1923:GLY:HA3	1.97	0.47
2:B:1977:ASN:H	2:B:1977:ASN:ND2	2.11	0.47
1:A:266:VAL:HG23	1:A:289:SER:HA	1.97	0.47
1:A:480:ILE:HG22	1:A:481:THR:N	2.28	0.47
1:A:637:TRP:NE1	1:A:680:MET:HG3	2.29	0.47
2:B:1755:HIS:CD2	2:B:1755:HIS:H	2.31	0.47
2:B:1755:HIS:HB3	2:B:1931:GLY:O	2.15	0.47
2:B:2179:GLY:HA2	2:B:2184:ALA:HB3	1.96	0.47
1:A:46:TYR:CD1	1:A:204:GLU:HG2	2.50	0.47
2:B:1888:SER:O	2:B:1890:TYR:N	2.47	0.47
2:B:2141:ASN:HD22	2:B:2142:PRO:HD2	1.80	0.47
1:A:383:VAL:HG22	1:A:462:LEU:CB	2.43	0.47
2:B:2091:GLN:HG3	2:B:2096:LEU:HD22	1.95	0.47
1:A:55:THR:HG22	1:A:62:ALA:HB3	1.96	0.47
1:A:68:TRP:CD1	1:A:68:TRP:N	2.83	0.47
2:B:1789:LEU:HD22	2:B:1823:MET:CB	2.45	0.47
2:B:1927:ASP:OD2	2:B:2013:LEU:CD1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2101:PHE:CD2	2:B:2151:LEU:HD13	2.50	0.47
2:B:2145:ILE:HD11	2:B:2171:LEU:HD21	1.97	0.47
2:B:2233:ASP:OD1	2:B:2304:ARG:NH1	2.48	0.47
1:A:449:LEU:HD12	1:A:449:LEU:N	2.19	0.46
2:B:1740:ASP:OD1	2:B:1744:THR:HG22	2.14	0.46
2:B:2002:ILE:O	2:B:2005:HIS:HB2	2.15	0.46
2:B:2211:HIS:O	2:B:2212:LEU:C	2.57	0.46
1:A:255:TRP:NE1	1:A:298:THR:OG1	2.47	0.46
2:B:2261:LEU:O	2:B:2309:HIS:N	2.47	0.46
3:C:2:NAG:N2	3:C:2:NAG:C5	2.78	0.46
1:A:89:LYS:HB2	1:A:89:LYS:HE2	1.46	0.46
2:B:1960:GLY:C	2:B:1961:HIS:HD2	2.23	0.46
2:B:1999:GLU:HB2	2:B:2006:LEU:HD21	1.96	0.46
2:B:2246:GLN:HB3	2:B:2320:ARG:HB2	1.97	0.46
2:B:1739:THR:HG22	2:B:1740:ASP:H	1.78	0.46
1:A:54:PHE:HA	1:A:62:ALA:O	2.14	0.46
1:A:141:LEU:O	1:A:142:LYS:C	2.59	0.46
1:A:588:THR:HA	1:A:591:ILE:HG22	1.98	0.46
2:B:1793:GLU:O	2:B:1794:GLU:CB	2.58	0.46
1:A:141:LEU:C	1:A:143:GLU:N	2.72	0.46
1:A:457:VAL:O	1:A:556:LYS:HD3	2.16	0.46
2:B:1920:ALA:HB1	2:B:1923:GLY:HA2	1.98	0.46
2:B:1932:LEU:HD12	2:B:2013:LEU:O	2.15	0.46
1:A:152:LEU:O	1:A:152:LEU:HD23	2.16	0.46
1:A:386:ILE:O	1:A:465:PHE:HA	2.16	0.46
2:B:1951:GLU:C	2:B:1953:ILE:H	2.20	0.46
1:A:49:THR:C	1:A:50:LEU:HG	2.40	0.46
1:A:526:PRO:O	1:A:528:CYS:N	2.48	0.46
2:B:2086:THR:HG22	2:B:2162:LEU:HD11	1.98	0.46
1:A:410:GLN:HG3	1:A:418:ARG:HH12	1.80	0.46
1:A:489:ARG:HH11	1:A:489:ARG:CG	2.29	0.46
2:B:2276:GLN:HG3	2:B:2298:ASP:CG	2.41	0.46
1:A:543:LEU:HD21	1:A:643:GLY:HA3	1.98	0.45
1:A:137:VAL:HG12	2:B:2329:GLN:OE1	2.16	0.45
1:A:408:LYS:HB3	1:A:622:PHE:CZ	2.50	0.45
1:A:14:TRP:HA	1:A:14:TRP:CE3	2.51	0.45
1:A:178:VAL:C	1:A:179:CYS:SG	2.99	0.45
1:A:237:TYR:HD2	1:A:242:LEU:HG	1.80	0.45
1:A:287:GLU:HB3	1:A:671:PHE:CD2	2.51	0.45
1:A:680:MET:HE3	1:A:680:MET:HA	1.98	0.45
2:B:1737:GLU:HG3	2:B:1747:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1829:GLU:CD	2:B:1833:LYS:HE2	2.41	0.45
2:B:2105:TYR:CD2	2:B:2144:ILE:HG23	2.51	0.45
2:B:2321:MET:HG2	2:B:2322:GLU:N	2.31	0.45
1:A:472:PRO:O	1:A:537:VAL:HG11	2.17	0.45
1:A:516:THR:O	1:A:517:VAL:C	2.59	0.45
2:B:2224:ASN:HB3	2:B:2317:ILE:CD1	2.45	0.45
1:A:116:ASP:HB2	1:A:123:LYS:HE2	1.98	0.45
2:B:2049:LYS:C	2:B:2051:ALA:N	2.74	0.45
1:A:522:THR:O	1:A:525:ASP:HB2	2.17	0.45
2:B:1771:ILE:HD12	2:B:1817:TRP:CZ2	2.51	0.45
2:B:2102:ILE:HD12	2:B:2102:ILE:O	2.16	0.45
1:A:243:PRO:O	1:A:244:GLY:C	2.60	0.45
1:A:312:ILE:HD11	1:A:315:HIS:ND1	2.31	0.45
1:A:533:TYR:CE1	1:A:549:GLY:C	2.94	0.45
1:A:574:ILE:O	1:A:639:ILE:HA	2.17	0.45
1:A:671:PHE:O	1:A:672:PRO:C	2.59	0.45
1:A:412:LEU:O	1:A:413:ASN:C	2.59	0.45
7:A:3333:EDO:H21	2:B:1973:MET:HE1	1.99	0.45
2:B:1750:GLY:HA3	2:B:2116:ARG:HH11	1.80	0.45
2:B:1920:ALA:HB1	2:B:1923:GLY:CA	2.47	0.45
1:A:50:LEU:HD23	1:A:171:GLY:HA3	1.98	0.45
1:A:403:ASP:O	1:A:405:ARG:HG2	2.16	0.45
2:B:1977:ASN:ND2	2:B:1977:ASN:N	2.64	0.45
2:B:1982:VAL:HG23	2:B:1982:VAL:O	2.17	0.45
2:B:2086:THR:HG22	2:B:2162:LEU:CD1	2.47	0.45
1:A:103:VAL:HG12	1:A:140:VAL:HG12	1.99	0.44
1:A:203:ASP:HA	1:A:230:LYS:HG3	1.98	0.44
1:A:408:LYS:CB	1:A:622:PHE:CZ	3.00	0.44
2:B:1776:ARG:HD3	2:B:1812:THR:HG23	1.99	0.44
1:A:114:TYR:N	1:A:114:TYR:CD1	2.86	0.44
1:A:669:THR:HG21	2:B:1979:TYR:HB3	1.99	0.44
2:B:1966:ARG:HD3	2:B:1985:THR:HB	1.98	0.44
2:B:2193:SER:HB3	2:B:2229:TRP:CD2	2.52	0.44
2:B:2286:ASN:ND2	2:B:2286:ASN:N	2.64	0.44
2:B:2025:LEU:HD11	2:B:2081:ILE:HG22	1.99	0.44
1:A:578:VAL:H	1:A:644:ALA:HA	1.83	0.44
1:A:431:TYR:HE2	1:A:437:LYS:HA	1.82	0.44
2:B:1891:PHE:HD1	2:B:1893:GLU:HG2	1.83	0.44
2:B:2087:GLN:HG3	2:B:2088:GLY:H	1.82	0.44
1:A:147:MET:HE3	2:B:1964:THR:HG23	1.99	0.44
1:A:194:LYS:HD2	1:A:256:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1782:PRO:O	2:B:1783:TYR:HD1	2.01	0.44
2:B:1927:ASP:OD2	2:B:2013:LEU:HD13	2.18	0.44
2:B:2064:THR:CG2	2:B:2066:GLU:HG2	2.43	0.44
2:B:2152:HIS:CD2	2:B:2152:HIS:N	2.86	0.44
1:A:276:PHE:O	1:A:277:LEU:HG	2.18	0.44
2:B:2252:LEU:HB3	2:B:2253:THR:H	1.52	0.44
1:A:45:VAL:O	1:A:47:LYS:HE3	2.17	0.44
1:A:522:THR:HB	1:A:523:LYS:NZ	2.33	0.44
1:A:530:THR:HB	1:A:638:TYR:HB3	1.99	0.44
1:A:642:ILE:C	1:A:644:ALA:H	2.26	0.44
2:B:1920:ALA:HB1	2:B:1923:GLY:C	2.42	0.44
2:B:1920:ALA:HB1	2:B:1924:TYR:N	2.33	0.44
2:B:1946:SER:CB	2:B:1978:LEU:HB3	2.45	0.44
2:B:1947:MET:O	2:B:1952:ASN:ND2	2.51	0.44
2:B:2029:SER:C	2:B:2031:HIS:H	2.26	0.44
2:B:2214:GLY:H	2:B:2217:ASN:ND2	2.09	0.44
1:A:426:VAL:HG13	1:A:426:VAL:O	2.18	0.44
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.66	0.44
2:B:1763:ILE:HB	2:B:1855:LEU:HD12	2.00	0.44
2:B:2061:ALA:CB	2:B:2163:ARG:HG3	2.34	0.44
2:B:2123:LEU:HD22	2:B:2124:MET:N	2.32	0.44
1:A:289:SER:HB2	1:A:290:PRO:HD2	1.99	0.43
1:A:637:TRP:CD1	1:A:680:MET:HG3	2.53	0.43
2:B:1767:VAL:C	2:B:1769:ASP:H	2.26	0.43
2:B:1879:PHE:CE1	2:B:1881:THR:OG1	2.70	0.43
1:A:643:GLY:CA	1:A:645:GLN:HE22	2.31	0.43
2:B:1781:ARG:CG	2:B:1889:TRP:CE3	3.02	0.43
1:A:49:THR:HG21	1:A:94:HIS:HD1	1.83	0.43
1:A:209:HIS:CE1	1:A:229:PRO:HG3	2.43	0.43
1:A:253:VAL:CG2	1:A:300:LEU:HD11	2.48	0.43
1:A:460:THR:HG23	1:A:514:THR:CG2	2.46	0.43
2:B:2232:VAL:HG13	2:B:2306:LEU:HB3	2.01	0.43
2:B:2251:LEU:O	2:B:2252:LEU:O	2.35	0.43
2:B:2256:TYR:H	2:B:2314:VAL:HG11	1.81	0.43
1:A:197:LEU:CD2	1:A:308:LEU:HD11	2.49	0.43
1:A:276:PHE:CE2	1:A:286:LEU:HG	2.53	0.43
1:A:317:HIS:C	1:A:319:GLY:N	2.76	0.43
1:A:486:LEU:HD23	1:A:487:TYR:HE1	1.79	0.43
2:B:1995:ILE:HD11	2:B:2013:LEU:HD23	1.99	0.43
1:A:230:LYS:HB3	1:A:230:LYS:HZ2	1.84	0.43
1:A:309:PHE:CD1	1:A:309:PHE:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ASP:O	1:A:606:PRO:C	2.62	0.43
2:B:2123:LEU:HD22	2:B:2123:LEU:C	2.43	0.43
1:A:141:LEU:HD12	1:A:144:ASN:HD22	1.84	0.43
2:B:2025:LEU:HD23	2:B:2025:LEU:HA	1.72	0.43
1:A:88:LEU:HG	1:A:89:LYS:N	2.33	0.43
1:A:157:SER:HA	1:A:176:LEU:H	1.83	0.43
1:A:269:ILE:N	1:A:269:ILE:CD1	2.78	0.43
2:B:1729:GLN:O	2:B:1730:PHE:HB2	2.18	0.43
2:B:2074:ASP:C	2:B:2076:LEU:H	2.26	0.43
1:A:279:ARG:HG2	2:B:1971:TYR:CZ	2.54	0.43
2:B:1845:LYS:C	2:B:1847:VAL:H	2.26	0.43
1:A:158:TYR:CE1	1:A:174:GLY:HA3	2.53	0.43
1:A:279:ARG:NH1	1:A:279:ARG:HG3	2.33	0.43
1:A:408:LYS:CB	1:A:622:PHE:CE1	3.00	0.43
1:A:530:THR:HA	1:A:552:LEU:HD23	2.00	0.43
2:B:1865:PRO:C	2:B:1867:HIS:H	2.25	0.43
1:A:299:LEU:HD21	1:A:301:MET:HE1	1.99	0.42
1:A:501:PHE:HA	1:A:502:PRO:HD3	1.71	0.42
1:A:55:THR:H	1:A:62:ALA:HB3	1.84	0.42
2:B:1766:GLU:O	2:B:1769:ASP:HB2	2.20	0.42
2:B:1781:ARG:CB	2:B:1889:TRP:CZ3	3.00	0.42
2:B:1858:CYS:CB	2:B:1862:THR:HG21	2.44	0.42
1:A:100:ALA:HB2	1:A:138:TRP:CE2	2.52	0.42
1:A:668:LEU:HD12	1:A:669:THR:H	1.84	0.42
2:B:1867:HIS:O	2:B:1867:HIS:ND1	2.52	0.42
1:A:386:ILE:HD12	1:A:463:ILE:HG23	2.01	0.42
2:B:1762:TYR:CD1	2:B:1854:PRO:HG2	2.54	0.42
2:B:2152:HIS:HA	2:B:2153:PRO:HD2	1.91	0.42
1:A:204:GLU:O	1:A:209:HIS:HB2	2.19	0.42
1:A:680:MET:HA	1:A:680:MET:CE	2.49	0.42
2:B:1926:MET:H	2:B:2009:GLY:HA3	1.84	0.42
1:A:384:HIS:ND1	1:A:384:HIS:N	2.67	0.42
1:A:540:GLU:N	1:A:540:GLU:CD	2.78	0.42
2:B:1963:PHE:CD2	2:B:1986:VAL:HG11	2.55	0.42
2:B:2098:ILE:HG13	2:B:2161:THR:O	2.20	0.42
1:A:306:PHE:CE2	1:A:326:VAL:CG1	2.97	0.42
1:A:403:ASP:C	1:A:405:ARG:N	2.78	0.42
2:B:1752:LEU:HD21	2:B:2118:ASN:HA	2.02	0.42
2:B:1949:SER:C	2:B:1951:GLU:H	2.28	0.42
2:B:2157:SER:C	2:B:2158:ILE:HG12	2.37	0.42
2:B:1870:GLN:CG	2:B:1871:VAL:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ALA:HB2	1:A:408:LYS:HE3	2.02	0.42
1:A:597:ASN:HA	1:A:598:PRO:HD3	1.56	0.42
2:B:1794:GLU:O	2:B:1795:ASP:C	2.62	0.42
2:B:1874:GLN:NE2	2:B:1934:MET:HA	2.35	0.42
2:B:1874:GLN:HE22	2:B:1934:MET:HA	1.85	0.42
2:B:1805:ASN:HB2	2:B:1813:LYS:HE3	2.02	0.42
2:B:1845:LYS:HD3	2:B:1889:TRP:CD1	2.55	0.42
2:B:2196:PHE:HD2	2:B:2203:TRP:CD1	2.38	0.42
1:A:263:THR:HB	2:B:2004:GLU:OE1	2.20	0.41
1:A:309:PHE:CB	1:A:321:GLU:HB3	2.49	0.41
2:B:2123:LEU:HD13	2:B:2123:LEU:O	2.19	0.41
2:B:1734:VAL:CG1	2:B:1735:PHE:N	2.75	0.41
1:A:463:ILE:HG21	1:A:475:ILE:CD1	2.51	0.41
1:A:697:PHE:O	1:A:700:ARG:N	2.42	0.41
2:B:2111:LYS:HB2	2:B:2111:LYS:HE2	1.83	0.41
2:B:2150:ARG:HG2	2:B:2152:HIS:NE2	2.35	0.41
2:B:2255:MET:HB3	2:B:2316:GLN:HB2	2.02	0.41
1:A:110:GLU:OE2	1:A:114:TYR:OH	2.37	0.41
1:A:643:GLY:O	1:A:645:GLN:OE1	2.38	0.41
1:A:87:THR:HG23	1:A:135:THR:HG23	2.02	0.41
1:A:163:ASP:HB3	1:A:166:LYS:CB	2.44	0.41
1:A:320:MET:C	1:A:321:GLU:HG2	2.45	0.41
1:A:379:PRO:HA	1:A:556:LYS:NZ	2.35	0.41
1:A:660:HIS:O	1:A:661:LYS:CD	2.68	0.41
2:B:1764:ARG:HG2	2:B:1764:ARG:NH1	2.34	0.41
1:A:622:PHE:C	1:A:624:SER:N	2.78	0.41
2:B:1933:VAL:O	2:B:1933:VAL:CG1	2.68	0.41
2:B:1961:HIS:HB3	2:B:1988:MET:HE2	2.03	0.41
2:B:1989:LEU:HA	2:B:1990:PRO:HD3	1.88	0.41
2:B:2263:SER:OG	2:B:2309:HIS:CE1	2.73	0.41
1:A:407:TYR:CD1	1:A:407:TYR:O	2.74	0.41
1:A:419:ILE:HG22	1:A:594:PHE:HB3	1.99	0.41
2:B:1709:TYR:N	2:B:1709:TYR:HD1	2.16	0.41
2:B:1733:VAL:HG11	2:B:1783:TYR:HE2	1.86	0.41
2:B:1781:ARG:CG	2:B:1889:TRP:HE3	2.32	0.41
2:B:1919:HIS:C	2:B:2010:MET:HE2	2.45	0.41
2:B:1960:GLY:C	2:B:1961:HIS:CD2	2.99	0.41
2:B:1994:GLY:O	2:B:2015:LEU:HD12	2.20	0.41
2:B:2007:HIS:CD2	2:B:2007:HIS:N	2.88	0.41
1:A:80:VAL:CG2	1:A:181:GLU:OE1	2.68	0.41
1:A:636:TYR:CE1	1:A:679:PHE:CD1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2035:PHE:CG	2:B:2036:GLN:N	2.87	0.41
2:B:2061:ALA:HB2	2:B:2163:ARG:CG	2.34	0.41
2:B:2179:GLY:CA	2:B:2184:ALA:HB3	2.50	0.41
1:A:4:ARG:HG3	1:A:85:VAL:O	2.20	0.41
1:A:10:VAL:HG21	1:A:54:PHE:HZ	1.86	0.41
1:A:67:PRO:CB	1:A:243:PRO:HG2	2.49	0.41
1:A:197:LEU:HD21	1:A:308:LEU:HD11	2.02	0.41
1:A:687:LEU:HD23	1:A:687:LEU:HA	1.98	0.41
2:B:1739:THR:HG21	2:B:1745:GLN:CB	2.50	0.41
2:B:1783:TYR:O	2:B:1807:VAL:HG23	2.21	0.41
2:B:1820:GLN:H	2:B:1823:MET:CG	2.34	0.41
2:B:2010:MET:O	2:B:2011:SER:C	2.63	0.41
2:B:2288:ASP:OD1	2:B:2288:ASP:N	2.54	0.41
1:A:63:LYS:HD2	1:A:63:LYS:N	2.36	0.41
1:A:317:HIS:O	1:A:319:GLY:N	2.54	0.41
1:A:668:LEU:HD12	1:A:669:THR:N	2.36	0.41
1:A:701:GLY:O	1:A:702:MET:HB3	2.21	0.41
2:B:1862:THR:HG23	2:B:1863:LEU:N	2.35	0.41
2:B:2037:ILE:HG12	2:B:2073:VAL:HG22	2.03	0.41
2:B:2077:ALA:HA	2:B:2078:PRO:HD2	1.94	0.41
2:B:2179:GLY:O	2:B:2180:MET:C	2.64	0.41
1:A:8:GLY:HA3	1:A:54:PHE:HE2	1.86	0.40
1:A:55:THR:O	1:A:56:ASP:O	2.39	0.40
1:A:56:ASP:OD1	1:A:56:ASP:C	2.64	0.40
1:A:301:MET:HB3	1:A:302:ASP:OD1	2.20	0.40
2:B:1891:PHE:CD1	2:B:1893:GLU:HG2	2.56	0.40
2:B:2164:MET:HE3	2:B:2164:MET:HB2	1.94	0.40
2:B:2217:ASN:O	2:B:2218:ALA:HB2	2.20	0.40
2:B:2241:THR:O	2:B:2297:LEU:N	2.54	0.40
1:A:116:ASP:O	1:A:117:GLN:CB	2.68	0.40
1:A:249:HIS:O	1:A:300:LEU:O	2.40	0.40
1:A:443:GLN:HB3	1:A:446:SER:H	1.86	0.40
2:B:1735:PHE:HB2	2:B:1760:GLY:HA3	2.02	0.40
2:B:2116:ARG:HG3	2:B:2120:THR:HG23	2.03	0.40
2:B:2171:LEU:HD23	2:B:2171:LEU:HA	1.46	0.40
1:A:541:ARG:HD2	1:A:583:ARG:O	2.21	0.40
1:A:625:LEU:HD12	1:A:625:LEU:C	2.45	0.40
2:B:1707:TRP:O	2:B:1729:GLN:O	2.39	0.40
2:B:2204:SER:HA	2:B:2205:PRO:HD2	1.82	0.40
2:B:2275:PHE:HE1	2:B:2280:VAL:HG22	1.86	0.40
1:A:90:ASN:OD1	1:A:90:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:TRP:HH2	2:B:1792:TYR:CE2	2.40	0.40
2:B:1937:ASP:O	2:B:1938:GLN:C	2.64	0.40
4:D:3:BMA:H62	4:D:5:BMA:H2	1.71	0.40
1:A:150:ASP:O	1:A:151:PRO:O	2.39	0.40
1:A:664:TYR:CE2	2:B:1822:HIS:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	602/760 (79%)	440 (73%)	97 (16%)	65 (11%)	0	7
2	B	598/685 (87%)	445 (74%)	101 (17%)	52 (9%)	0	10
All	All	1200/1445 (83%)	885 (74%)	198 (16%)	117 (10%)	0	9

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	46	TYR
1	A	54	PHE
1	A	56	ASP
1	A	62	ALA
1	A	69	MET
1	A	70	GLY
1	A	151	PRO
1	A	164	LEU
1	A	187	GLU
1	A	230	LYS
1	A	240	ARG
1	A	290	PRO

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Mol	Chain	Res	Type
1	A	397	PRO
1	A	402	PRO
1	A	528	CYS
1	A	539	MET
1	A	606	PRO
1	A	672	PRO
1	A	696	ASP
1	A	698	ARG
2	B	1711	MET
2	B	1790	ILE
2	B	1794	GLU
2	B	1804	LYS
2	B	1827	LYS
2	B	1871	VAL
2	B	1892	THR
2	B	1893	GLU
2	B	1952	ASN
2	B	1966	ARG
2	B	2046	TRP
2	B	2049	LYS
2	B	2077	ALA
2	B	2118	ASN
2	B	2133	SER
2	B	2194	SER
2	B	2210	LEU
2	B	2252	LEU
2	B	2298	ASP
2	B	2331	LEU
1	A	2	THR
1	A	67	PRO
1	A	81	TYR
1	A	90	ASN
1	A	232	HIS
1	A	243	PRO
1	A	244	GLY
1	A	245	LEU
1	A	279	ARG
1	A	410	GLN
1	A	413	ASN
1	A	420	GLY
1	A	447	GLY
1	A	469	ALA

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Mol	Chain	Res	Type
1	A	490	ARG
1	A	600	GLY
1	A	601	VAL
1	A	623	ASP
1	A	702	MET
2	B	1729	GLN
2	B	1730	PHE
2	B	1752	LEU
2	B	1786	TYR
2	B	1866	ALA
2	B	1889	TRP
2	B	1915	ASN
2	B	1967	LYS
2	B	2003	GLY
2	B	2117	GLY
2	B	2212	LEU
1	A	127	LYS
1	A	242	LEU
1	A	299	LEU
1	A	318	ASP
1	A	326	VAL
1	A	403	ASP
1	A	527	ARG
1	A	593	ARG
1	A	632	HIS
1	A	645	GLN
1	A	662	MET
2	B	1829	GLU
2	B	1867	HIS
2	B	1913	LYS
2	B	1991	SER
2	B	2067	PRO
2	B	2119	SER
2	B	2183	LYS
2	B	2290	PHE
1	A	148	ALA
1	A	239	ASN
1	A	302	ASP
1	A	598	PRO
1	A	599	ALA
2	B	2035	PHE
2	B	2061	ALA

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Mol	Chain	Res	Type
2	B	2132	SER
2	B	2218	ALA
1	A	63	LYS
1	A	406	SER
1	A	646	THR
2	B	1968	LYS
2	B	2187	ASP
2	B	2291	THR
2	B	2321	MET
1	A	52	VAL
1	A	597	ASN
1	A	622	PHE
2	B	1748	TYR
2	B	2193	SER
1	A	477	PRO
2	B	2158	ILE
1	A	264	PRO
1	A	472	PRO
2	B	1809	PRO
2	B	1850	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

7 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	1.22	2 (14%)	17,19,21	2.26	7 (41%)
3	NAG	C	2	3	14,14,15	0.66	0	17,19,21	2.16	5 (29%)
4	NAG	D	1	2,4	14,14,15	0.82	0	17,19,21	2.17	6 (35%)
4	NAG	D	2	4	14,14,15	1.28	3 (21%)	17,19,21	3.03	8 (47%)
4	BMA	D	3	4	11,11,12	0.85	0	15,15,17	1.55	2 (13%)
4	BMA	D	4	4	11,11,12	0.93	1 (9%)	15,15,17	1.48	2 (13%)
4	BMA	D	5	4	11,11,12	0.73	0	15,15,17	1.05	1 (6%)

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	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	BMA	D	4	4	-	2/2/19/22	0/1/1/1
4	BMA	D	5	4	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	2.77	1.56	1.52
4	D	2	NAG	C1-C2	2.76	1.56	1.52
4	D	2	NAG	C2-N2	2.60	1.50	1.46
4	D	4	BMA	C2-C3	2.33	1.56	1.52
3	C	1	NAG	C3-C2	2.09	1.56	1.52
4	D	2	NAG	C3-C2	2.05	1.56	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C2-N2-C7	7.02	132.31	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C4-C3-C2	6.39	120.38	111.02
3	C	2	NAG	C2-N2-C7	5.47	130.23	122.90
3	C	2	NAG	C1-O5-C5	5.37	119.38	112.19
4	D	2	NAG	C1-O5-C5	4.97	118.84	112.19
3	C	1	NAG	C4-C3-C2	4.61	117.78	111.02
4	D	1	NAG	C8-C7-N2	4.56	123.69	116.12
3	C	1	NAG	C2-N2-C7	4.14	128.44	122.90
4	D	3	BMA	C3-C4-C5	4.02	117.52	110.23
4	D	4	BMA	C2-C3-C4	3.52	117.04	110.86
3	C	1	NAG	C1-O5-C5	3.43	116.78	112.19
4	D	1	NAG	O5-C1-C2	-3.37	106.07	111.29
4	D	1	NAG	C2-N2-C7	3.37	127.42	122.90
4	D	4	BMA	C1-C2-C3	3.29	114.44	109.64
4	D	1	NAG	O7-C7-C8	-3.10	116.53	122.05
4	D	1	NAG	C1-C2-N2	2.97	115.12	110.43
4	D	2	NAG	C1-C2-N2	2.86	114.95	110.43
4	D	1	NAG	C4-C3-C2	2.82	115.16	111.02
3	C	2	NAG	O5-C5-C6	2.82	113.14	107.66
4	D	2	NAG	O5-C1-C2	2.71	115.49	111.29
3	C	1	NAG	O5-C5-C4	2.62	117.21	110.83
4	D	5	BMA	C1-O5-C5	2.50	115.54	112.19
3	C	2	NAG	C1-C2-N2	2.42	114.25	110.43
3	C	1	NAG	O7-C7-C8	-2.29	117.98	122.05
4	D	2	NAG	O7-C7-C8	-2.25	118.05	122.05
3	C	1	NAG	C1-C2-N2	-2.24	106.91	110.43
3	C	1	NAG	O3-C3-C4	-2.17	105.26	110.38
4	D	2	NAG	O4-C4-C5	2.10	114.50	109.32
4	D	2	NAG	O3-C3-C4	-2.05	105.55	110.38
4	D	3	BMA	C1-O5-C5	2.00	114.87	112.19
3	C	2	NAG	O5-C1-C2	-2.00	108.19	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	BMA	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2

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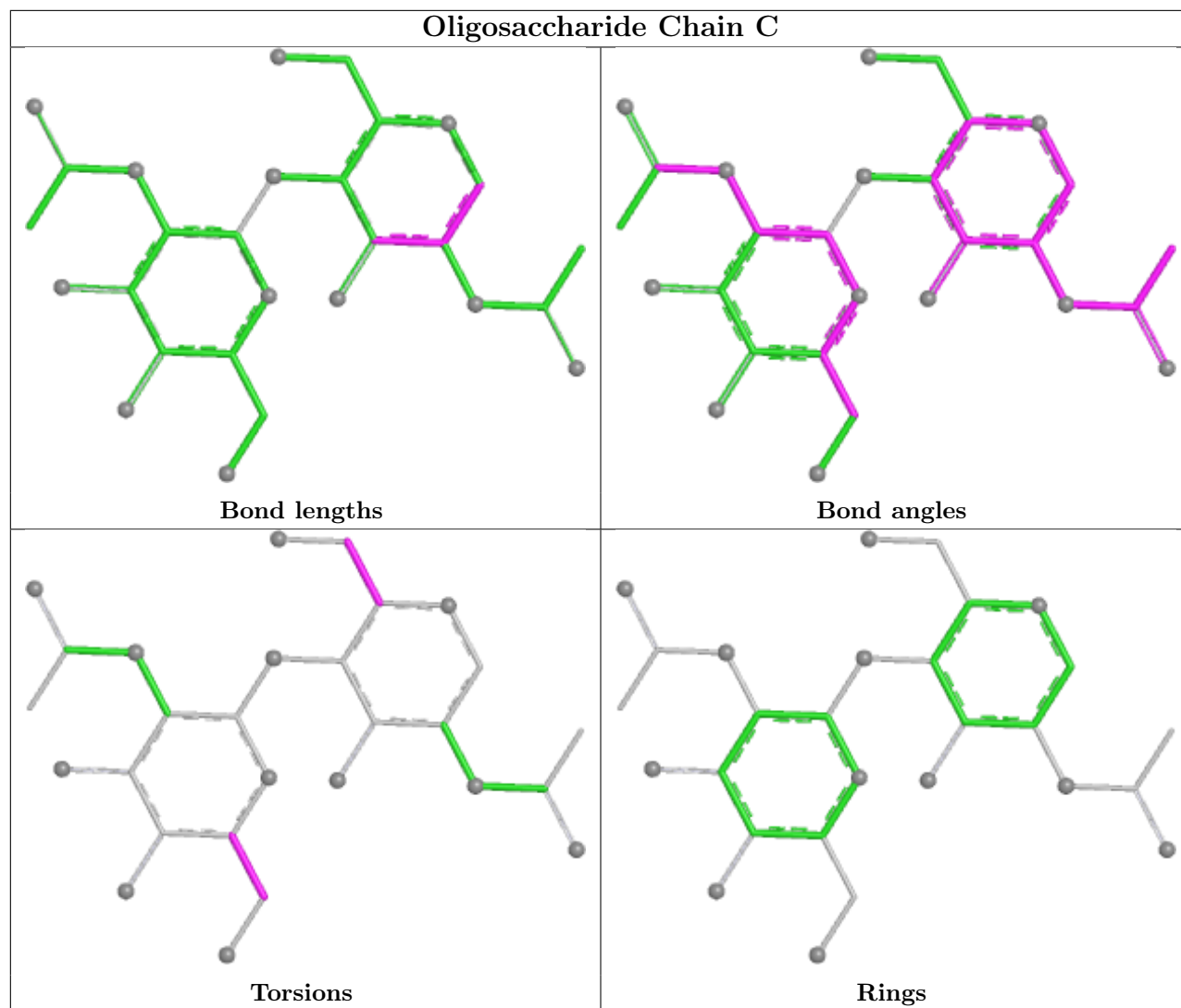
Mol	Chain	Res	Type	Atoms
4	D	5	BMA	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	4	BMA	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	5	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

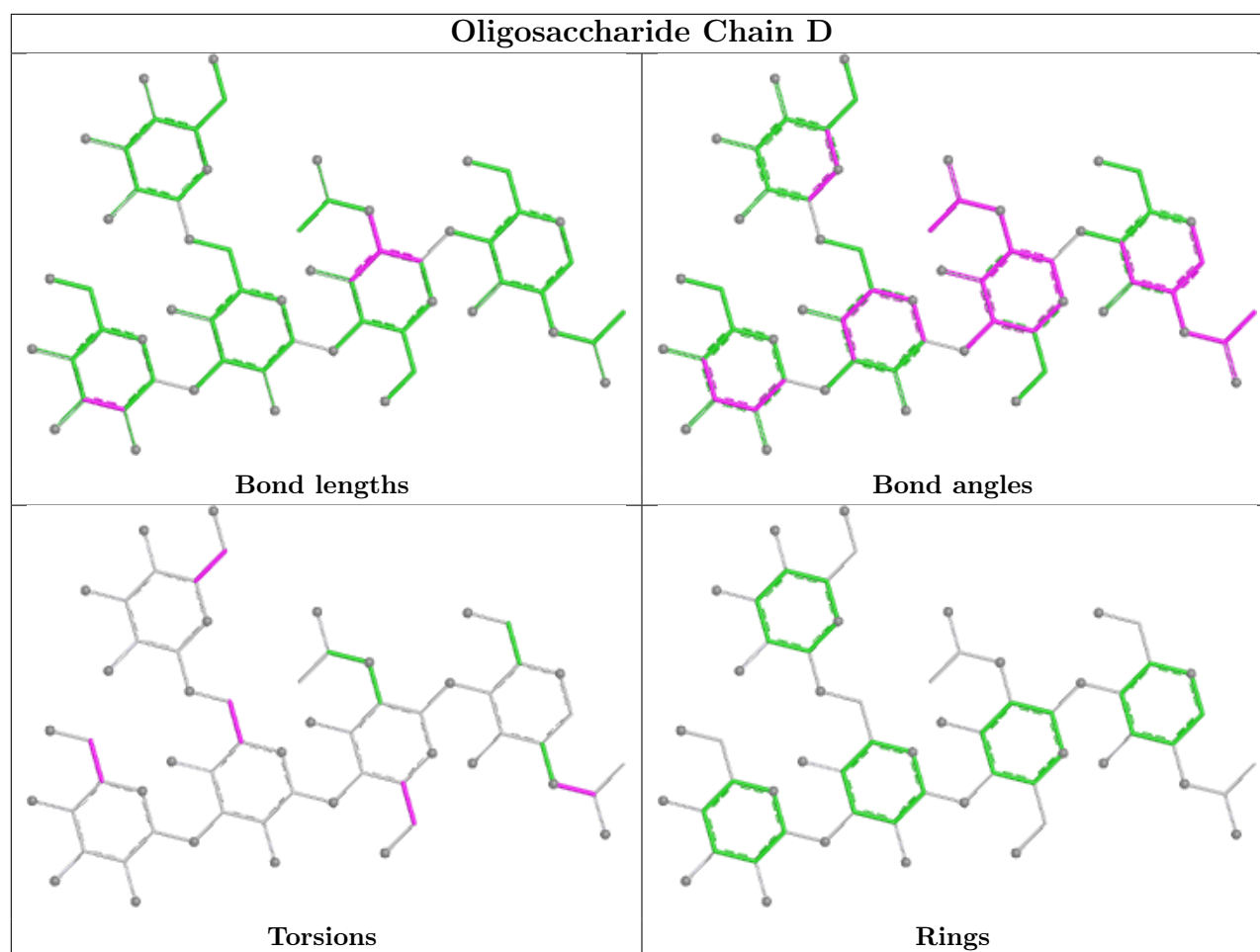
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
3	C	2	NAG	2	0
4	D	5	BMA	1	0
4	D	2	NAG	1	0
4	D	3	BMA	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.





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
7	EDO	B	3333	-	3,3,3	0.55	0	2,2,2	0.10	0
7	EDO	A	3333	-	3,3,3	0.45	0	2,2,2	0.31	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
7	EDO	B	3333	-	-	1/1/1/1	-
7	EDO	A	3333	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3333	EDO	O1-C1-C2-O2
7	B	3333	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3333	EDO	3	0

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	612/760 (80%)	-0.92	0 100 100	98, 154, 230, 309	0
2	B	606/685 (88%)	-0.92	0 100 100	99, 155, 213, 290	0
All	All	1218/1445 (84%)	-0.92	0 100 100	98, 154, 223, 309	0

There are no RSRZ outliers to report.

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](#)

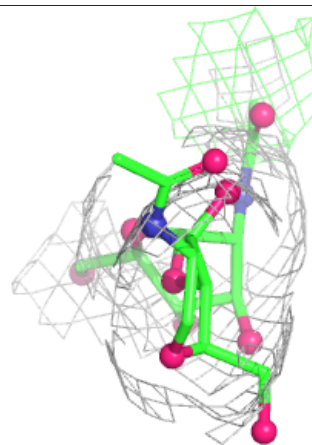
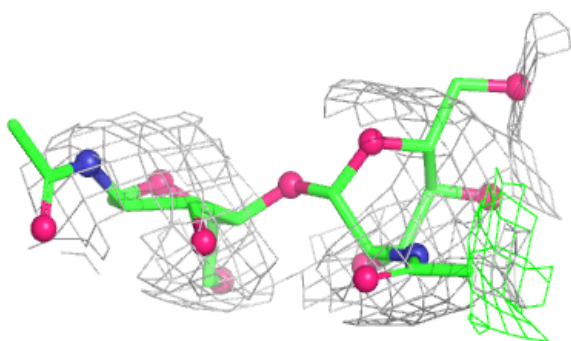
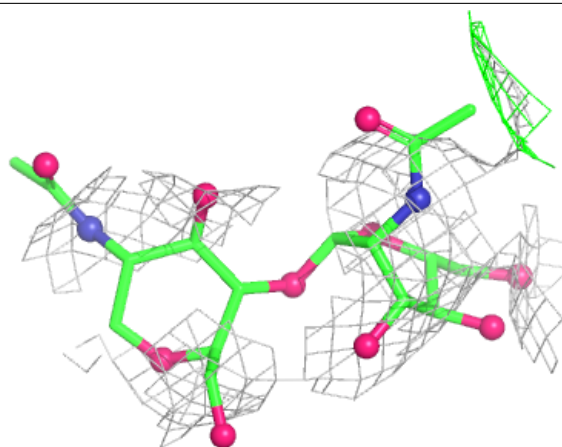
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

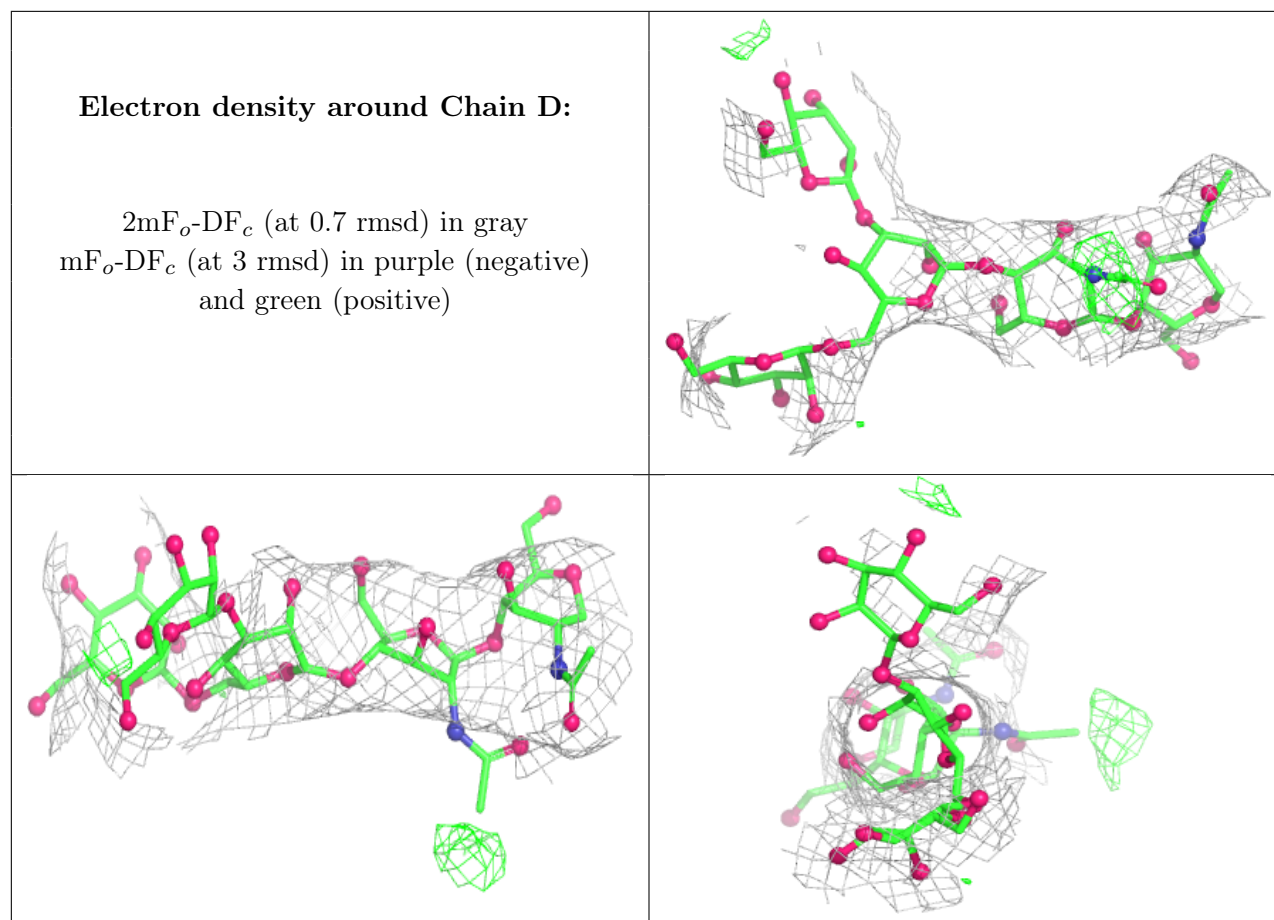
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.31	0.09	217,256,320,356	0
4	BMA	D	4	11/12	0.74	0.07	221,270,291,291	0
4	BMA	D	5	11/12	0.77	0.06	211,251,269,270	0
4	NAG	D	2	14/15	0.90	0.09	164,205,234,248	0
4	BMA	D	3	11/12	0.90	0.05	202,237,263,297	0
3	NAG	C	1	14/15	0.92	0.07	197,223,245,258	0
4	NAG	D	1	14/15	0.97	0.08	151,173,209,221	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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	B	3333	4/4	0.93	0.13	129,134,141,143	0
7	EDO	A	3333	4/4	0.94	0.13	170,174,186,187	0
5	ZN	A	800	1/1	0.99	0.02	144,144,144,144	0
6	CA	A	801	1/1	1.00	0.02	130,130,130,130	0
8	CU1	B	1	1/1	1.00	0.01	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.