



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:00 AM BST

PDB ID : 4BDV
Title : CRYSTAL STRUCTURE OF A TRUNCATED B-DOMAIN HUMAN FACTOR VIII
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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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

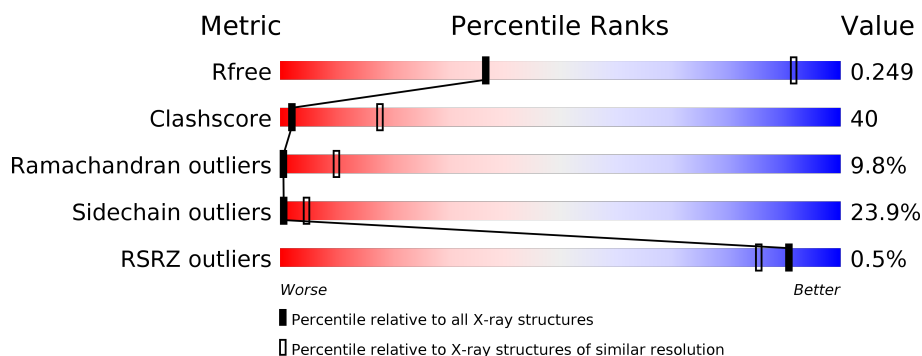
1 Overall quality at a glance

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}	130704	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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 on 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	<div> <div></div> <div>25% 38% 15% • 19%</div> </div>
2	B	685	<div> <div></div> <div>32% 41% 14% • 12%</div> </div>
3	C	2	<div> <div></div> <div>50% 50%</div> </div>
4	D	5	<div> <div></div> <div>20% 80%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	X	-	-	-
3	NAG	C	2	-	-	-	X
7	EDO	A	3333	-	-	-	X
7	EDO	B	3333	-	-	-	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.

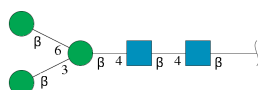
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	606	Total	C	N	O	S	0	0	0
			4929	3175	841	885	28			

- 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			

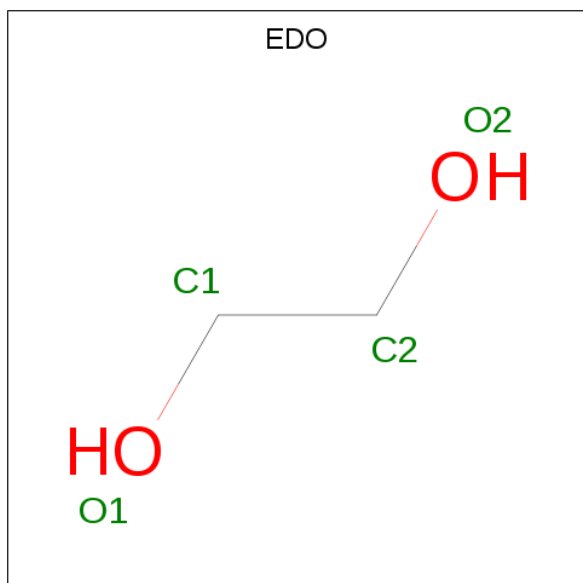
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: 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		

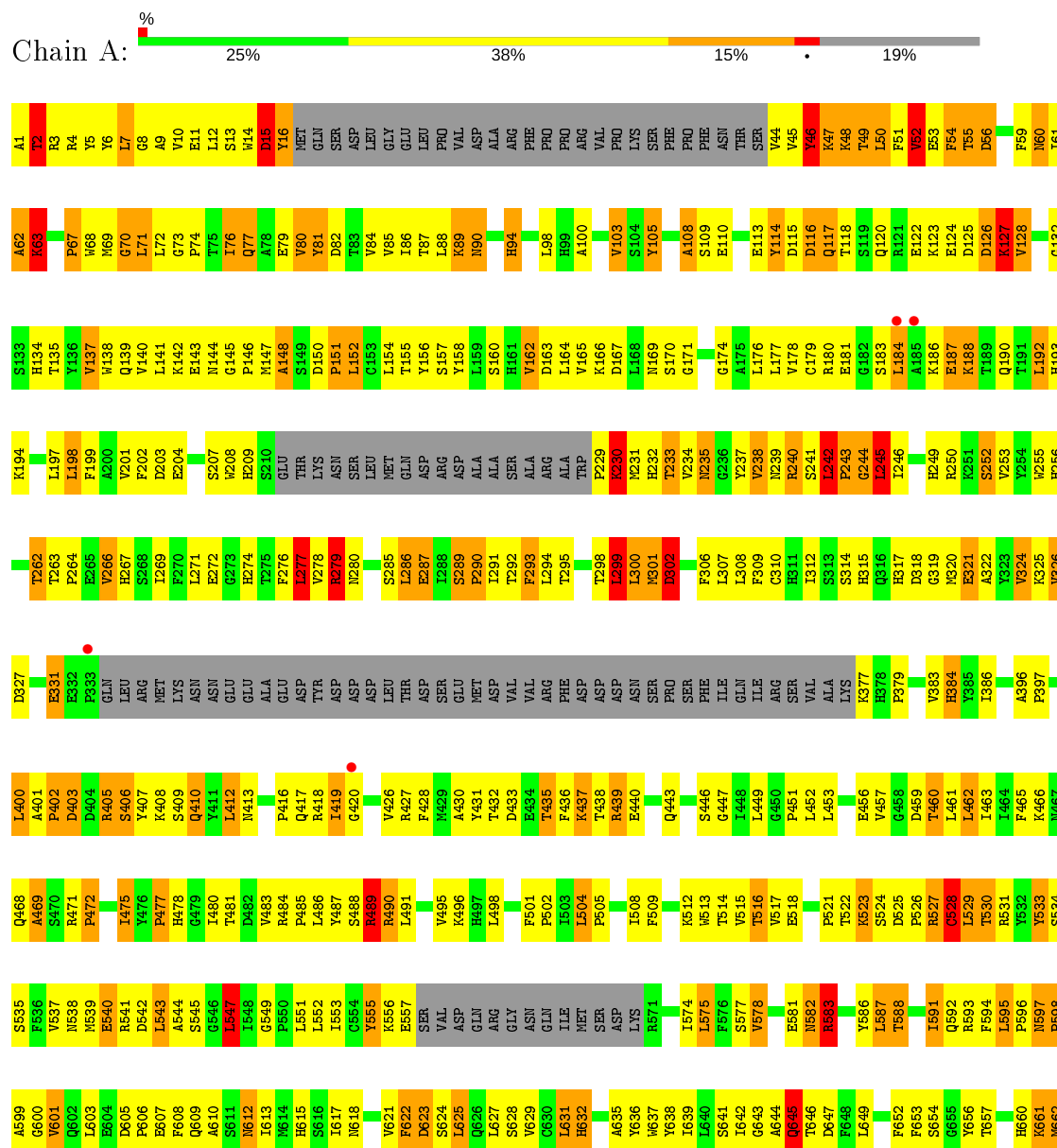
- Molecule 8 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

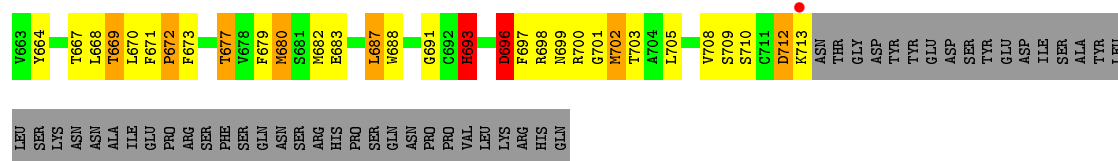
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cu	0	0
			1	1		

3 Residue-property plots

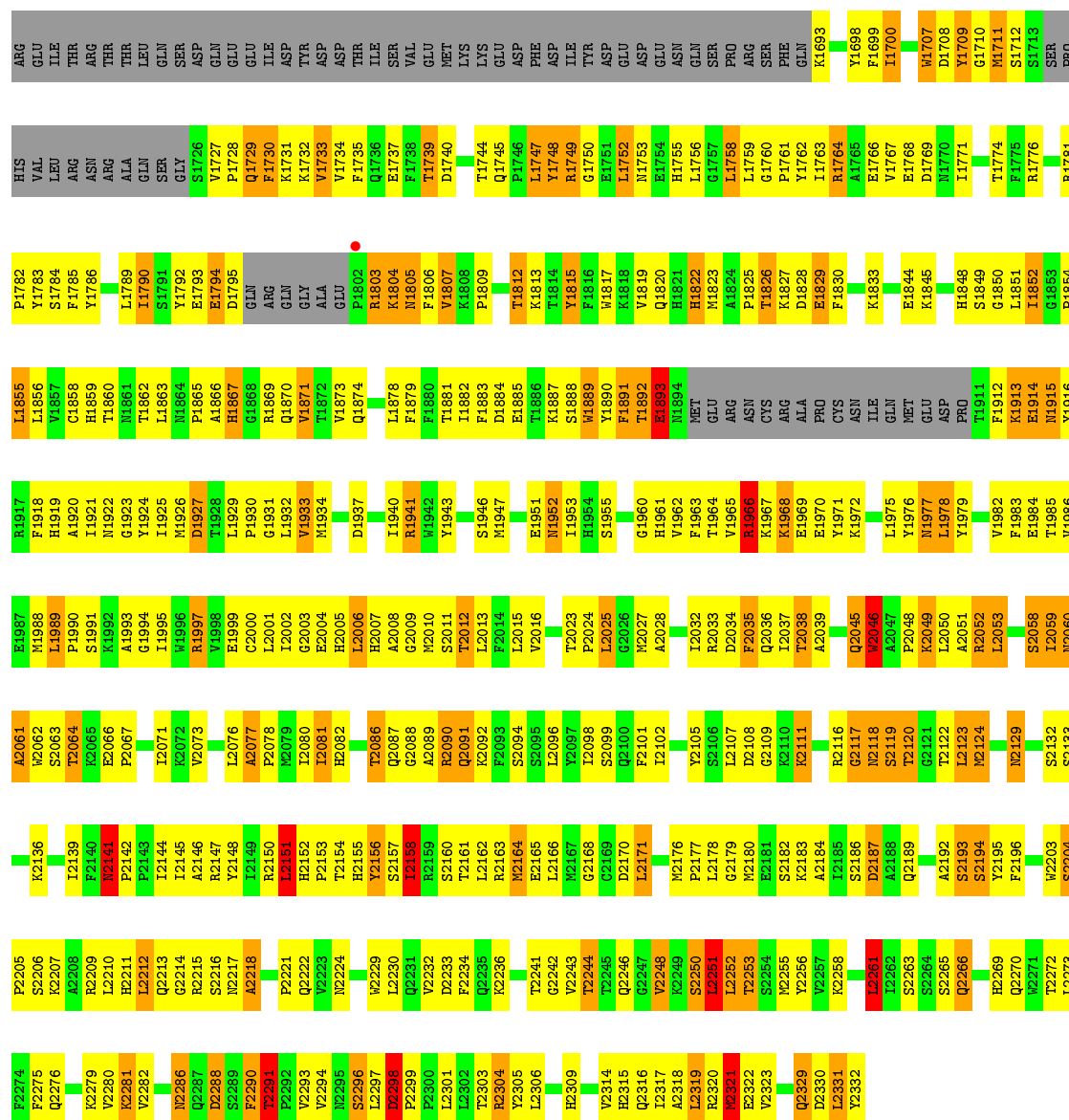
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: FACTOR VIIIA HEAVY CHAIN, 92 KDA ISOFORM, B DOMAIN





• Molecule 2: FACTOR VIIIA LIGHT CHAIN



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





- 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

Chain D:  20% 80%



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 19.99 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.98) 99.9 (19.99-3.98)	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 0.166 , 0.249	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)	0.26 , 120.0	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.68	1/5085 (0.0%)	1.00	18/6901 (0.3%)
2	B	0.64	0/5070	0.94	10/6864 (0.1%)
All	All	0.66	1/10155 (0.0%)	0.97	28/13765 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	TYR	N-CA	5.60	1.57	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2261	LEU	CA-CB-CG	-9.31	93.89	115.30
1	A	489	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	46	TYR	N-CA-C	7.75	131.93	111.00
1	A	184	LEU	CA-CB-CG	7.14	131.73	115.30
1	A	15	ASP	N-CA-C	7.09	130.16	111.00
1	A	489	ARG	NE-CZ-NH2	-6.99	116.80	120.30
2	B	1989	LEU	CA-CB-CG	6.74	130.79	115.30
2	B	2025	LEU	CA-CB-CG	-6.59	100.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LYS	N-CA-C	5.91	126.97	111.00
1	A	531	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	400	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	603	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	587	LEU	CA-CB-CG	5.67	128.34	115.30
2	B	2151	LEU	CA-CB-CG	5.58	128.14	115.30
2	B	2251	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	60	ASN	N-CA-C	5.50	125.84	111.00
2	B	2090	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	277	LEU	CA-CB-CG	-5.47	102.72	115.30
1	A	324	VAL	CB-CA-C	-5.42	101.11	111.40
1	A	242	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	286	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	547	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	192	LEU	CA-CB-CG	5.27	127.42	115.30
2	B	1728	PRO	N-CA-C	5.19	125.59	112.10
2	B	1727	VAL	N-CA-C	5.15	124.91	111.00
2	B	1852	ILE	CB-CA-C	-5.14	101.31	111.60
2	B	1749	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	412	LEU	CA-CB-CG	5.05	126.93	115.30

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	414	0
2	B	4929	0	4812	393	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	2	0
7	B	4	0	6	0	0
8	B	1	0	0	0	0
All	All	9973	0	9735	793	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 40.

All (793) 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:HD3	1:A:523:LYS:H	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	1.24	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
2:B:2266:GLN:HA	2:B:2266:GLN:NE2	1.79	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CD	1:A:523:LYS:H	1.83	0.89
1:A:146:PRO:HA	1:A:154:LEU:HD11	1.55	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: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
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:HD22	1:A:245:LEU:H	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:2314:VAL:HG13	2:B:2315:HIS:N	1.99	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
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
2:B:1870:GLN:HG3	2:B:1871:VAL:N	1.99	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: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:77:GLN:HG3	1:A:177:LEU:HB2	1.70	0.74
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
1:A:14:TRP:CD1	1:A:231:MET:HE1	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2156:TYR:N	2:B:2156:TYR:HD1	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
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:209:HIS:HE1	1:A:229:PRO:HG3	1.54	0.71
1:A:63:LYS:O	1:A:63:LYS:HG2	1.89	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
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:660:HIS:C	1:A:661:LYS:HD3	2.11	0.71
2:B:1739:THR:CG2	2:B:1740:ASP:N	2.54	0.71
1:A:471:ARG:CZ	1:A:471:ARG:HB2	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:1941:ARG:HD2	2:B:1943:TYR:CZ	2.25	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:1734:VAL:HG12	2:B:1735:PHE:N	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HD12	1:A:269:ILE:N	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
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:H	2:B:2286:ASN:ND2	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:2108:ASP:CG	2:B:2109:GLY:H	1.97	0.67
2:B:2141:ASN:CB	2:B:2142:PRO:HD2	2.25	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
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:61:ILE:CG1	1:A:63:LYS:HZ2	2.08	0.66
1:A:486:LEU:HD23	1:A:487:TYR:CE1	2.31	0.66
1:A:489:ARG:HH11	1:A:489:ARG:HG3	1.61	0.66
1:A:278:VAL:O	1:A:280:ASN:N	2.28	0.66
1:A:61:ILE:HG13	1:A:63:LYS:HZ2	1.61	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:331:GLU:H	1:A:331:GLU:CD	1.99	0.65
1:A:61:ILE:O	1:A:62:ALA:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:137:VAL:O	1:A:137:VAL:CG1	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
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
2:B:2182:SER:C	2:B:2184:ALA:H	2.02	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
2:B:2102:ILE:C	2:B:2102:ILE:HD12	2.20	0.61
1:A:661:LYS:O	1:A:661:LYS:HG2	2.01	0.61
1:A:682:MET:HG2	1:A:682:MET:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD12	1:A:141:LEU:H	1.67	0.60
2:B:1708:ASP:C	2:B:1709:TYR:CD1	2.75	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
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: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
1:A:82:ASP:O	1:A:140:VAL:HG22	2.03	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:H	2:B:1977:ASN:HD22	1.50	0.59
2:B:2006:LEU:C	2:B:2008:ALA:H	2.04	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:O	2:B:2291:THR:HG22	2.03	0.58
1:A:157:SER:HA	1:A:176:LEU:HB3	1.85	0.58
2:B:1893:GLU:CA	2:B:1893:GLU:OE1	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:405:ARG:HG3	1:A:406:SER:N	2.18	0.58
1:A:7:LEU:HD21	1:A:51:PHE:CD1	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2076:LEU:O	2:B:2077:ALA:HB2	2.02	0.58
1:A:269:ILE:HA	1:A:309:PHE:O	2.03	0.58
1:A:245:LEU:HB3	1:A:324:VAL:HA	1.85	0.58
1:A:62:ALA:N	1:A:63:LYS:HE3	2.11	0.58
2:B:1914:GLU:CD	2:B:1915:ASN:N	2.58	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: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:48:LYS:HA	1:A:208:TRP:HZ2	1.69	0.57
1:A:4:ARG:HD3	1:A:6:TYR:HE1	1.70	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
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
2:B:2108:ASP:CG	2:B:2109:GLY:N	2.59	0.57
1:A:105:TYR:CE1	1:A:110:GLU:HB2	2.40	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
2:B:2250:SER:C	2:B:2252:LEU:H	2.07	0.56
1:A:116:ASP:O	1:A:117:GLN:HB2	2.03	0.56
1:A:115:ASP:HB3	1:A:117:GLN:OE1	2.06	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:2023:THR:OG1	2:B:2024:PRO:CD	2.52	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:147:MET:HE2	2:B:1972:LYS:HB2	1.86	0.56
1:A:290:PRO:HB3	2:B:2002:ILE:HG21	1.86	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:230:LYS:HZ2	1:A:230:LYS:HB3	1.68	0.56
1:A:687:LEU:H	2:B:1803:ARG:HG3	1.71	0.56
1:A:50:LEU:HD22	1:A:71:LEU:HB2	1.88	0.56
1:A:693:HIS:CD2	1:A:693:HIS:O	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: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:HA	2:B:2281:LYS:HE2	1.88	0.55
1:A:45:VAL:C	1:A:47:LYS:HZ1	2.10	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: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
1:A:433:ASP:OD1	1:A:433:ASP:N	2.40	0.54
1:A:463:ILE:HG21	1:A:475:ILE:HD12	1.89	0.54
1:A:108:ALA:HA	1:A:125:ASP:OD1	2.08	0.54
1:A:80:VAL:O	1:A:81:TYR:CG	2.61	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:555:TYR:CD1	1:A:556:LYS:N	2.73	0.54
1:A:529:LEU:HA	1:A:677:THR:HG21	1.89	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
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
1:A:419:ILE:HG22	1:A:594:PHE:HB2	1.90	0.53
2:B:1826:THR:C	2:B:1828:ASP:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:B:2141:ASN:ND2	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
1:A:680:MET:HA	1:A:680:MET:HE3	1.90	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:405:ARG:CG	1:A:406:SER:N	2.72	0.53
1:A:308:LEU:HD23	1:A:322:ALA:O	2.09	0.53
1:A:6:TYR:CD2	1:A:56:ASP:O	2.62	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:2156:TYR:H	2:B:2156:TYR:HD1	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
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
2:B:2049:LYS:C	2:B:2051:ALA:H	2.11	0.52
2:B:2182:SER:C	2:B:2184:ALA:N	2.63	0.52
1:A:278:VAL:O	1:A:279:ARG:C	2.47	0.52
2:B:1789:LEU:HD22	2:B:1823:MET:HB3	1.91	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
1:A:468:GLN:O	1:A:469:ALA:HB2	2.08	0.52
2:B:2250:SER:C	2:B:2252:LEU:N	2.62	0.52
1:A:631:LEU:O	1:A:632:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:O	1:A:140:VAL:CG2	2.55	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:48:LYS:HZ3	1:A:231:MET:HE1	1.74	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: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
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
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
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
2:B:2129:ASN:OD1	2:B:2129:ASN:N	2.44	0.50
2:B:2151:LEU:HD12	2:B:2151:LEU:C	2.32	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
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:430:ALA:HB2	1:A:451:PRO:HG3	1.93	0.50
1:A:5:TYR:HE2	1:A:76:ILE:HB	1.77	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1764:ARG:HH11	2:B:1764:ARG:HG2	1.77	0.50
7:A:3333:EDO:H22	2:B:1977:ASN:ND2	2.27	0.50
1:A:291:ILE:HG22	2:B:1955:SER:CB	2.42	0.49
1:A:271:LEU:CD1	1:A:308:LEU:HB3	2.38	0.49
1:A:696:ASP:N	1:A:696:ASP:OD1	2.42	0.49
2:B:1709:TYR:HD2	2:B:1924:TYR:HA	1.77	0.49
2:B:1914:GLU:CD	2:B:1915:ASN:H	2.15	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:652:PHE:O	1:A:653:PHE:HB2	2.12	0.49
2:B:1888:SER:C	2:B:1890:TYR:H	2.15	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:128:VAL:CG1	1:A:132:GLY:O	2.59	0.49
1:A:63:LYS:O	1:A:63:LYS:CG	2.54	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:1934:MET:HE1	2:B:1940:ILE:HD13	1.95	0.49
2:B:2101:PHE:CE2	2:B:2151:LEU:HD22	2.48	0.49
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
1:A:702:MET:HG3	1:A:702:MET:O	2.13	0.49
2:B:2275:PHE:CE1	2:B:2280:VAL:HG22	2.48	0.49
1:A:245:LEU:CD2	1:A:245:LEU:N	2.76	0.49
2:B:2053:LEU:HA	2:B:2163:ARG:HB3	1.95	0.49
1:A:417:GLN:C	1:A:418:ARG:HG2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1888:SER:C	2:B:1890:TYR:N	2.67	0.49
2:B:2224:ASN:ND2	2:B:2317:ILE:HD12	2.23	0.49
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:461:LEU:HB2	1:A:513:TRP:HB2	1.95	0.48
1:A:453:LEU:CD1	1:A:453:LEU:N	2.76	0.48
1:A:6:TYR:HD2	1:A:56:ASP:O	1.95	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: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
2:B:2286:ASN:HA	2:B:2293:VAL:HG11	1.96	0.48
1:A:14:TRP:HD1	1:A:231:MET:CE	2.10	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: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
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
2:B:1825:PRO:HD3	2:B:1833:LYS:HB2	1.96	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
1:A:586:TYR:O	1:A:587:LEU:C	2.52	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:2117:GLY:O	2:B:2118:ASN:C	2.53	0.47
2:B:2214:GLY:N	2:B:2217:ASN:HD22	2.09	0.47
1:A:53:GLU:CD	1:A:74:PRO:HB3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD12	1:A:453:LEU:N	2.29	0.47
1:A:71:LEU:HD12	1:A:71:LEU:H	1.79	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: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
7:A:3333:EDO:H22	2:B:1977:ASN:HD21	1.78	0.47
1:A:581:GLU:HB2	1:A:612:ASN:O	2.14	0.47
1:A:645:GLN:HE21	1:A:645:GLN:HA	1.80	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: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:2179:GLY:HA2	2:B:2184:ALA:HB3	1.96	0.47
1:A:266:VAL:HG23	1:A:289:SER:HA	1.97	0.47
2:B:1755:HIS:H	2:B:1755:HIS:CD2	2.31	0.47
2:B:1755:HIS:HB3	2:B:1931:GLY:O	2.15	0.47
1:A:46:TYR:CD1	1:A:204:GLU:HG2	2.50	0.47
1:A:45:VAL:C	1:A:47:LYS:NZ	2.68	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
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
1:A:622:PHE:O	1:A:623:ASP:C	2.53	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
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:C5	3:C:2:NAG:N2	2.78	0.46
1:A:89:LYS:HE2	1:A:89:LYS:HB2	1.46	0.46
2:B:1999:GLU:HB2	2:B:2006:LEU:HD21	1.96	0.46
2:B:2192:ALA:C	2:B:2194:SER:H	2.19	0.46
2:B:2246:GLN:HB3	2:B:2320:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1739:THR:HG22	2:B:1740:ASP:H	1.78	0.46
2:B:1826:THR:C	2:B:1828:ASP:N	2.69	0.46
1:A:54:PHE:HA	1:A:62:ALA:O	2.14	0.46
1:A:56:ASP:OD2	1:A:59:PHE:C	2.54	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
2:B:2012:THR:C	2:B:2013:LEU:HD12	2.36	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:HD23	1:A:152:LEU:O	2.16	0.46
1:A:386:ILE:O	1:A:465:PHE:HA	2.16	0.46
1:A:526:PRO:O	1:A:528:CYS:N	2.48	0.46
1:A:596:PRO:O	1:A:597:ASN:C	2.53	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
1:A:543:LEU:HD21	1:A:643:GLY:HA3	1.98	0.45
1:A:120:GLN:C	1:A:122:GLU:N	2.69	0.45
1:A:137:VAL:HG12	2:B:2329:GLN:OE1	2.16	0.45
1:A:147:MET:O	1:A:148:ALA:C	2.55	0.45
1:A:48:LYS:NZ	1:A:231:MET:HE1	2.31	0.45
1:A:408:LYS:HB3	1:A:622:PHE:CZ	2.50	0.45
1:A:14:TRP:CE3	1:A:14:TRP:HA	2.51	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:643:GLY:O	1:A:645:GLN:CD	2.54	0.45
2:B:1737:GLU:HG3	2:B:1747:LEU:HB3	1.98	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:61:ILE:HG12	1:A:63:LYS:HZ2	1.79	0.45
2:B:2099:SER:HB3	2:B:2155:HIS:C	2.36	0.45
2:B:2176:MET:CE	2:B:2177:PRO:HD2	2.45	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
1:A:540:GLU:CD	1:A:540:GLU:H	2.20	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:O	2:B:2102:ILE:HD12	2.16	0.45
1:A:312:ILE:HD11	1:A:315:HIS:ND1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ILE:O	1:A:639:ILE:HA	2.17	0.45
2:B:1920:ALA:HB1	2:B:1923:GLY:CA	2.47	0.45
2:B:1750:GLY:HA3	2:B:2116:ARG:HH11	1.80	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
1:A:61:ILE:HG13	1:A:63:LYS:HZ1	1.76	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:120:GLN:C	1:A:122:GLU:H	2.19	0.44
1:A:194:LYS:HD2	1:A:256:HIS:NE2	2.33	0.44
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:N	2:B:2152:HIS:CD2	2.86	0.44
1:A:276:PHE:O	1:A:277:LEU:HG	2.18	0.44
1:A:403:ASP:C	1:A:405:ARG:H	2.20	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
2:B:1920:ALA:HB1	2:B:1924:TYR:N	2.33	0.44
2:B:1947:MET:O	2:B:1952:ASN:ND2	2.51	0.44
2:B:1946:SER:CB	2:B:1978:LEU:HB3	2.45	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:HA	1:A:670:LEU:HD23	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1763:ILE:HB	2:B:1855:LEU:HD12	2.00	0.44
2:B:2123:LEU:HD22	2:B:2124:MET:N	2.32	0.44
2:B:2061:ALA:CB	2:B:2163:ARG:HG3	2.34	0.44
1:A:289:SER:HB2	1:A:290:PRO:HD2	1.99	0.43
1:A:489:ARG:O	1:A:490:ARG:C	2.55	0.43
1:A:637:TRP:CD1	1:A:680:MET:HG3	2.53	0.43
2:B:1879:PHE:CE1	2:B:1881:THR:OG1	2.70	0.43
1:A:272:GLU:C	1:A:274:HIS:H	2.21	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: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
1:A:49:THR:HG21	1:A:94:HIS:HD1	1.83	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
2:B:2232:VAL:HG13	2:B:2306:LEU:HB3	2.01	0.43
1:A:276:PHE:CE2	1:A:286:LEU:HG	2.53	0.43
1:A:197:LEU:CD2	1:A:308:LEU:HD11	2.49	0.43
1:A:486:LEU:HD23	1:A:487:TYR:HE1	1.79	0.43
1:A:712:ASP:O	1:A:713:LYS:C	2.57	0.43
2:B:1995:ILE:HD11	2:B:2013:LEU:HD23	1.99	0.43
1:A:309:PHE:CD1	1:A:309:PHE:N	2.86	0.43
1:A:68:TRP:C	1:A:70:GLY:N	2.71	0.43
1:A:141:LEU:HD12	1:A:144:ASN:HD22	1.84	0.43
2:B:2025:LEU:HA	2:B:2025:LEU:HD23	1.72	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
1:A:88:LEU:HG	1:A:89:LYS:N	2.33	0.43
2:B:1729:GLN:O	2:B:1730:PHE:HB2	2.18	0.43
1:A:279:ARG:HG2	2:B:1971:TYR:CZ	2.54	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:530:THR:HA	1:A:552:LEU:HD23	2.00	0.43
1:A:408:LYS:CB	1:A:622:PHE:CE1	3.00	0.43
1:A:501:PHE:HA	1:A:502:PRO:HD3	1.71	0.42
2:B:2118:ASN:O	2:B:2119:SER:C	2.57	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:1858:CYS:CB	2:B:1862:THR:HG21	2.44	0.42
2:B:1781:ARG:CB	2:B:1889:TRP:CZ3	3.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:CE	2:B:1972:LYS:HB2	2.48	0.42
2:B:2102:ILE:CD1	2:B:2102:ILE:C	2.87	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:ND1	2:B:1867:HIS:O	2.52	0.42
2:B:2035:PHE:CG	2:B:2036:GLN:N	2.87	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:CE	1:A:680:MET:HA	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
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
2:B:1752:LEU:HD21	2:B:2118:ASN:HA	2.02	0.42
2:B:1870:GLN:CG	2:B:1871:VAL:N	2.70	0.42
1:A:147:MET:HE2	2:B:1972:LYS:NZ	2.34	0.42
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:1874:GLN:HE22	2:B:1934:MET:HA	1.85	0.42
2:B:1874:GLN:NE2	2:B:1934:MET:HA	2.35	0.42
2:B:2211:HIS:O	2:B:2212:LEU:C	2.57	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:309:PHE:CB	1:A:321:GLU:HB3	2.49	0.41
1:A:263:THR:HB	2:B:2004:GLU:OE1	2.20	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
2:B:1960:GLY:C	2:B:1961:HIS:HD2	2.23	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:HE2	2:B:2111:LYS:HB2	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:141:LEU:O	1:A:142:LYS:C	2.59	0.41
1:A:643:GLY:O	1:A:645:GLN:OE1	2.38	0.41
2:B:1711:MET:CG	2:B:1712:SER:N	2.77	0.41
1:A:87:THR:HG23	1:A:135:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:C	1:A:143:GLU:N	2.72	0.41
1:A:163:ASP:HB3	1:A:166:LYS:CB	2.44	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:NH1	2:B:1764:ARG:HG2	2.34	0.41
2:B:1933:VAL:CG1	2:B:1933:VAL:O	2.68	0.41
2:B:1951:GLU:C	2:B:1953:ILE:H	2.20	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
1:A:49:THR:C	1:A:50:LEU:HG	2.40	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:1934:MET:HE1	2:B:1940:ILE:CD1	2.50	0.41
2:B:1994:GLY:O	2:B:2015:LEU:HD12	2.20	0.41
2:B:2007:HIS:N	2:B:2007:HIS:CD2	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
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
2:B:2276:GLN:HG3	2:B:2298:ASP:CG	2.41	0.41
1:A:67:PRO:CB	1:A:243:PRO:HG2	2.49	0.41
1:A:4:ARG:HG3	1:A:85:VAL:O	2.20	0.41
2:B:1820:GLN:H	2:B:1823:MET:CG	2.34	0.41
2:B:2288:ASP:OD1	2:B:2288:ASP:N	2.54	0.41
1:A:10:VAL:HG21	1:A:54:PHE:HZ	1.86	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:1862:THR:HG23	2:B:1863:LEU:N	2.35	0.41
2:B:2006:LEU:C	2:B:2008:ALA:N	2.72	0.41
1:A:178:VAL:C	1:A:179:CYS:SG	2.99	0.41
1:A:317:HIS:O	1:A:319:GLY:N	2.54	0.41
1:A:63:LYS:N	1:A:63:LYS:HD2	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2176:MET:HE3	2:B:2177:PRO:HD2	2.03	0.41
1:A:301:MET:HB3	1:A:302:ASP:OD1	2.20	0.40
1:A:516:THR:O	1:A:517:VAL:C	2.59	0.40
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
2:B:1829:GLU:CD	2:B:1833:LYS:HE2	2.41	0.40
2:B:1891:PHE:CD1	2:B:1893:GLU:HG2	2.56	0.40
2:B:2049:LYS:C	2:B:2051:ALA:N	2.74	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:HA	2:B:2171:LEU:HD23	1.46	0.40
2:B:2291:THR:CG2	2:B:2291:THR:O	2.68	0.40
1:A:147:MET:CE	2:B:1972:LYS:NZ	2.84	0.40
1:A:147:MET:HE2	2:B:1972:LYS:CE	2.51	0.40
1:A:541:ARG:HD2	1:A:583:ARG:O	2.21	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:688:TRP:HH2	2:B:1792:TYR:CE2	2.40	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:243:PRO:O	1:A:244:GLY:C	2.60	0.40
1:A:533:TYR:CE1	1:A:549:GLY:C	2.94	0.40
1:A:664:TYR:CE2	2:B:1822:HIS:HA	2.56	0.40
2:B:1934:MET:HB2	2:B:1934:MET:HE3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	8
2	B	598/685 (87%)	445 (74%)	101 (17%)	52 (9%)	1	12
All	All	1200/1445 (83%)	885 (74%)	198 (16%)	117 (10%)	0	10

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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	544/680 (80%)	404 (74%)	140 (26%)	0	4
2	B	539/613 (88%)	420 (78%)	119 (22%)	1	6
All	All	1083/1293 (84%)	824 (76%)	259 (24%)	0	5

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	ARG
1	A	7	LEU
1	A	12	LEU
1	A	13	SER
1	A	16	TYR
1	A	44	VAL
1	A	47	LYS
1	A	48	LYS
1	A	49	THR
1	A	50	LEU
1	A	52	VAL
1	A	55	THR
1	A	63	LYS
1	A	71	LEU
1	A	72	LEU
1	A	76	ILE
1	A	77	GLN
1	A	80	VAL
1	A	84	VAL
1	A	86	ILE
1	A	89	LYS
1	A	94	HIS
1	A	98	LEU
1	A	103	VAL
1	A	105	TYR
1	A	114	TYR

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Mol	Chain	Res	Type
1	A	116	ASP
1	A	117	GLN
1	A	124	GLU
1	A	126	ASP
1	A	127	LYS
1	A	128	VAL
1	A	134	HIS
1	A	137	VAL
1	A	139	GLN
1	A	152	LEU
1	A	162	VAL
1	A	188	LYS
1	A	192	LEU
1	A	193	HIS
1	A	198	LEU
1	A	201	VAL
1	A	230	LYS
1	A	233	THR
1	A	235	ASN
1	A	238	VAL
1	A	242	LEU
1	A	245	LEU
1	A	246	ILE
1	A	250	ARG
1	A	252	SER
1	A	262	THR
1	A	266	VAL
1	A	277	LEU
1	A	279	ARG
1	A	285	SER
1	A	287	GLU
1	A	289	SER
1	A	292	THR
1	A	293	PHE
1	A	294	LEU
1	A	295	THR
1	A	299	LEU
1	A	300	LEU
1	A	301	MET
1	A	302	ASP
1	A	314	SER
1	A	320	MET

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Mol	Chain	Res	Type
1	A	321	GLU
1	A	325	LYS
1	A	327	ASP
1	A	331	GLU
1	A	377	LYS
1	A	384	HIS
1	A	405	ARG
1	A	412	LEU
1	A	419	ILE
1	A	427	ARG
1	A	432	THR
1	A	435	THR
1	A	437	LYS
1	A	439	ARG
1	A	440	GLU
1	A	452	LEU
1	A	460	THR
1	A	462	LEU
1	A	475	ILE
1	A	478	HIS
1	A	488	SER
1	A	489	ARG
1	A	491	LEU
1	A	496	LYS
1	A	498	LEU
1	A	504	LEU
1	A	516	THR
1	A	518	GLU
1	A	523	LYS
1	A	524	SER
1	A	528	CYS
1	A	529	LEU
1	A	530	THR
1	A	533	TYR
1	A	540	GLU
1	A	543	LEU
1	A	547	LEU
1	A	555	TYR
1	A	557	GLU
1	A	575	LEU
1	A	578	VAL
1	A	582	ASN

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Mol	Chain	Res	Type
1	A	583	ARG
1	A	588	THR
1	A	591	ILE
1	A	595	LEU
1	A	601	VAL
1	A	607	GLU
1	A	612	ASN
1	A	617	ILE
1	A	625	LEU
1	A	627	LEU
1	A	628	SER
1	A	629	VAL
1	A	631	LEU
1	A	645	GLN
1	A	654	SER
1	A	656	TYR
1	A	657	THR
1	A	661	LYS
1	A	669	THR
1	A	677	THR
1	A	680	MET
1	A	683	GLU
1	A	687	LEU
1	A	693	HIS
1	A	696	ASP
1	A	708	VAL
1	A	709	SER
1	A	710	SER
1	A	712	ASP
2	B	1693	LYS
2	B	1700	ILE
2	B	1707	TRP
2	B	1709	TYR
2	B	1731	LYS
2	B	1733	VAL
2	B	1739	THR
2	B	1747	LEU
2	B	1748	TYR
2	B	1749	ARG
2	B	1753	ASN
2	B	1758	LEU
2	B	1764	ARG

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Mol	Chain	Res	Type
2	B	1774	THR
2	B	1784	SER
2	B	1795	ASP
2	B	1803	ARG
2	B	1805	ASN
2	B	1806	PHE
2	B	1807	VAL
2	B	1812	THR
2	B	1815	TYR
2	B	1822	HIS
2	B	1826	THR
2	B	1844	GLU
2	B	1852	ILE
2	B	1855	LEU
2	B	1856	LEU
2	B	1860	THR
2	B	1873	VAL
2	B	1887	LYS
2	B	1891	PHE
2	B	1893	GLU
2	B	1914	GLU
2	B	1916	TYR
2	B	1927	ASP
2	B	1933	VAL
2	B	1937	ASP
2	B	1941	ARG
2	B	1962	VAL
2	B	1964	THR
2	B	1965	VAL
2	B	1966	ARG
2	B	1969	GLU
2	B	1977	ASN
2	B	1978	LEU
2	B	1983	PHE
2	B	1988	MET
2	B	1997	ARG
2	B	2001	LEU
2	B	2006	LEU
2	B	2012	THR
2	B	2033	ARG
2	B	2038	THR
2	B	2045	GLN

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Mol	Chain	Res	Type
2	B	2046	TRP
2	B	2052	ARG
2	B	2053	LEU
2	B	2058	SER
2	B	2059	ILE
2	B	2060	ASN
2	B	2064	THR
2	B	2081	ILE
2	B	2086	THR
2	B	2090	ARG
2	B	2091	GLN
2	B	2092	LYS
2	B	2094	SER
2	B	2107	LEU
2	B	2111	LYS
2	B	2120	THR
2	B	2122	THR
2	B	2123	LEU
2	B	2124	MET
2	B	2129	ASN
2	B	2136	LYS
2	B	2139	ILE
2	B	2141	ASN
2	B	2151	LEU
2	B	2154	THR
2	B	2156	TYR
2	B	2158	ILE
2	B	2164	MET
2	B	2170	ASP
2	B	2171	LEU
2	B	2187	ASP
2	B	2204	SER
2	B	2206	SER
2	B	2213	GLN
2	B	2215	ARG
2	B	2222	GLN
2	B	2236	LYS
2	B	2243	VAL
2	B	2244	THR
2	B	2248	VAL
2	B	2250	SER
2	B	2251	LEU

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Mol	Chain	Res	Type
2	B	2253	THR
2	B	2258	LYS
2	B	2261	LEU
2	B	2266	GLN
2	B	2269	HIS
2	B	2270	GLN
2	B	2272	THR
2	B	2279	LYS
2	B	2281	LYS
2	B	2282	VAL
2	B	2286	ASN
2	B	2288	ASP
2	B	2290	PHE
2	B	2291	THR
2	B	2296	SER
2	B	2298	ASP
2	B	2301	LEU
2	B	2304	ARG
2	B	2319	LEU
2	B	2321	MET
2	B	2329	GLN
2	B	2332	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	144	ASN
1	A	169	ASN
1	A	190	GLN
1	A	193	HIS
1	A	209	HIS
1	A	235	ASN
1	A	280	ASN
1	A	305	GLN
1	A	316	GLN
1	A	582	ASN
1	A	609	GLN
1	A	645	GLN
1	A	693	HIS
2	B	1729	GLN
2	B	1745	GLN

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Mol	Chain	Res	Type
2	B	1755	HIS
2	B	1805	ASN
2	B	1822	HIS
2	B	1848	HIS
2	B	1870	GLN
2	B	1894	ASN
2	B	1950	ASN
2	B	1952	ASN
2	B	1954	HIS
2	B	1957	HIS
2	B	1961	HIS
2	B	1977	ASN
2	B	2007	HIS
2	B	2045	GLN
2	B	2082	HIS
2	B	2141	ASN
2	B	2211	HIS
2	B	2217	ASN
2	B	2222	GLN
2	B	2224	ASN
2	B	2235	GLN
2	B	2266	GLN
2	B	2309	HIS
2	B	2315	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,3	14,14,15	1.17	2 (14%)	17,19,21	2.25	8 (47%)
3	NAG	C	2	3	14,14,15	0.64	0	17,19,21	2.18	4 (23%)
4	NAG	D	1	2,4	14,14,15	0.81	0	17,19,21	2.12	6 (35%)
4	NAG	D	2	4	14,14,15	1.22	3 (21%)	17,19,21	2.95	8 (47%)
4	BMA	D	3	4	11,11,12	0.87	0	15,15,17	1.63	2 (13%)
4	BMA	D	4	4	11,11,12	0.96	1 (9%)	15,15,17	1.64	3 (20%)
4	BMA	D	5	4	11,11,12	0.75	0	15,15,17	1.10	2 (13%)

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	1,3	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	2.53	1.56	1.52
4	D	2	NAG	C1-C2	2.52	1.56	1.52
4	D	2	NAG	C2-N2	2.49	1.50	1.46
4	D	4	BMA	C2-C3	2.40	1.56	1.52
3	C	1	NAG	C3-C2	2.06	1.56	1.52
4	D	2	NAG	C3-C2	2.02	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C2-N2-C7	6.61	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	C1-O5-C5	5.31	119.38	112.19
3	C	2	NAG	C2-N2-C7	5.14	130.23	122.90
4	D	2	NAG	C1-O5-C5	4.91	118.84	112.19
3	C	1	NAG	C4-C3-C2	4.61	117.78	111.02
4	D	1	NAG	C8-C7-N2	4.48	123.69	116.10
4	D	3	BMA	C3-C4-C5	4.08	117.52	110.24
3	C	1	NAG	C2-N2-C7	3.89	128.44	122.90
4	D	4	BMA	C1-C2-C3	3.88	114.44	109.67
3	C	2	NAG	O5-C5-C6	3.79	113.14	107.20
4	D	4	BMA	C2-C3-C4	3.55	117.04	110.89
3	C	1	NAG	C1-O5-C5	3.39	116.78	112.19
4	D	1	NAG	O5-C1-C2	-3.30	106.07	111.29
4	D	1	NAG	C2-N2-C7	3.17	127.42	122.90
4	D	1	NAG	O7-C7-C8	-2.97	116.53	122.06
4	D	1	NAG	C4-C3-C2	2.82	115.16	111.02
4	D	1	NAG	C1-C2-N2	2.71	115.12	110.49
4	D	2	NAG	O5-C1-C2	2.66	115.49	111.29
3	C	1	NAG	O5-C5-C4	2.62	117.21	110.83
4	D	2	NAG	C1-C2-N2	2.61	114.95	110.49
4	D	5	BMA	C1-O5-C5	2.47	115.54	112.19
4	D	3	BMA	C1-C2-C3	-2.32	106.81	109.67
3	C	1	NAG	O3-C3-C4	-2.20	105.26	110.35
3	C	2	NAG	C1-C2-N2	2.20	114.25	110.49
3	C	1	NAG	O7-C7-C8	-2.19	117.98	122.06
4	D	2	NAG	O7-C7-C8	-2.16	118.05	122.06
4	D	5	BMA	O3-C3-C2	2.15	114.11	109.99
4	D	4	BMA	O5-C5-C6	2.14	110.56	107.20
3	C	1	NAG	C1-C2-N2	-2.10	106.91	110.49
4	D	2	NAG	O4-C4-C5	2.09	114.50	109.30
4	D	2	NAG	O3-C3-C4	-2.08	105.55	110.35
3	C	1	NAG	O5-C5-C6	2.06	110.44	107.20

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

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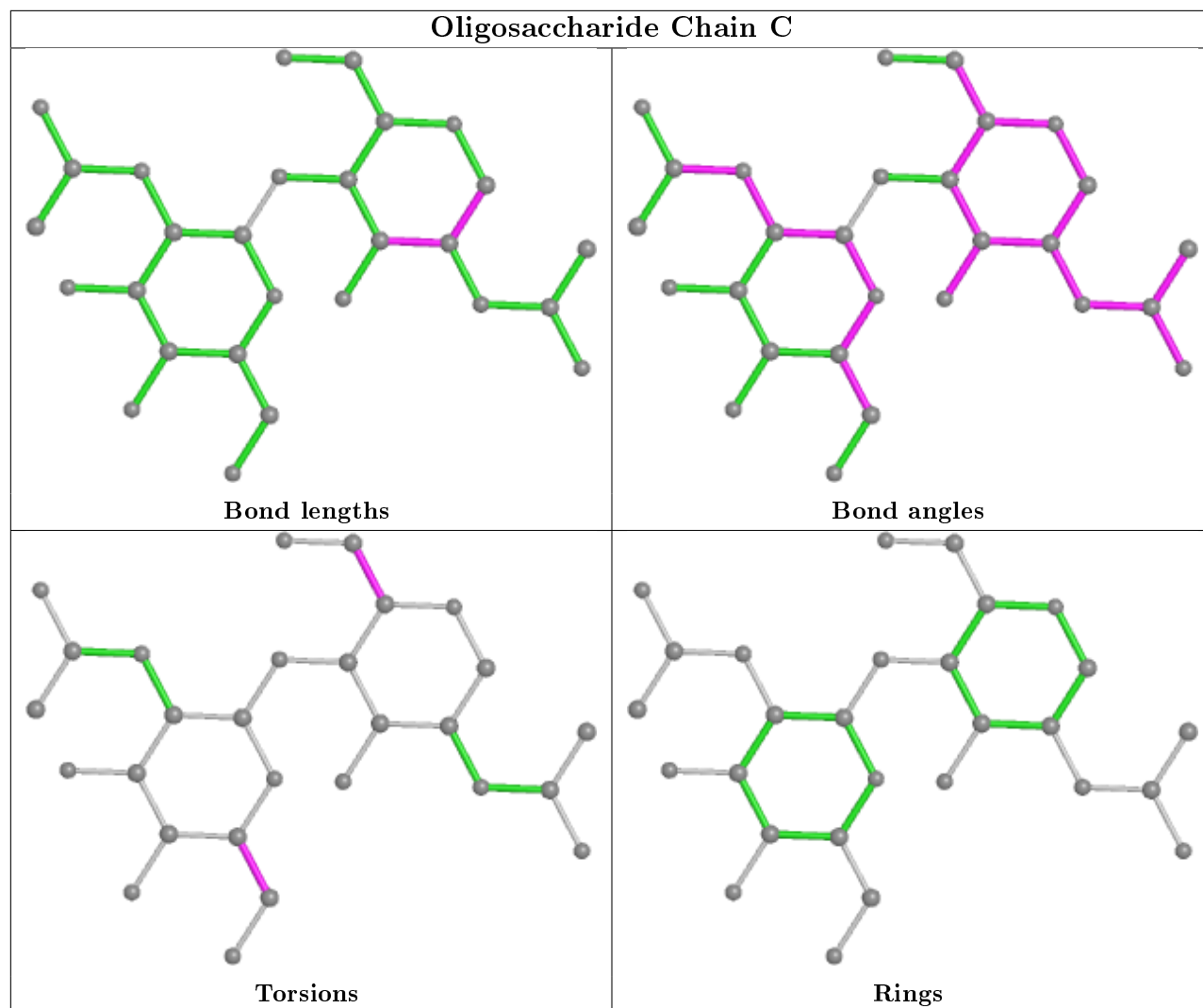
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C4-C5-C6-O6
4	D	5	BMA	C4-C5-C6-O6
4	D	4	BMA	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	5	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

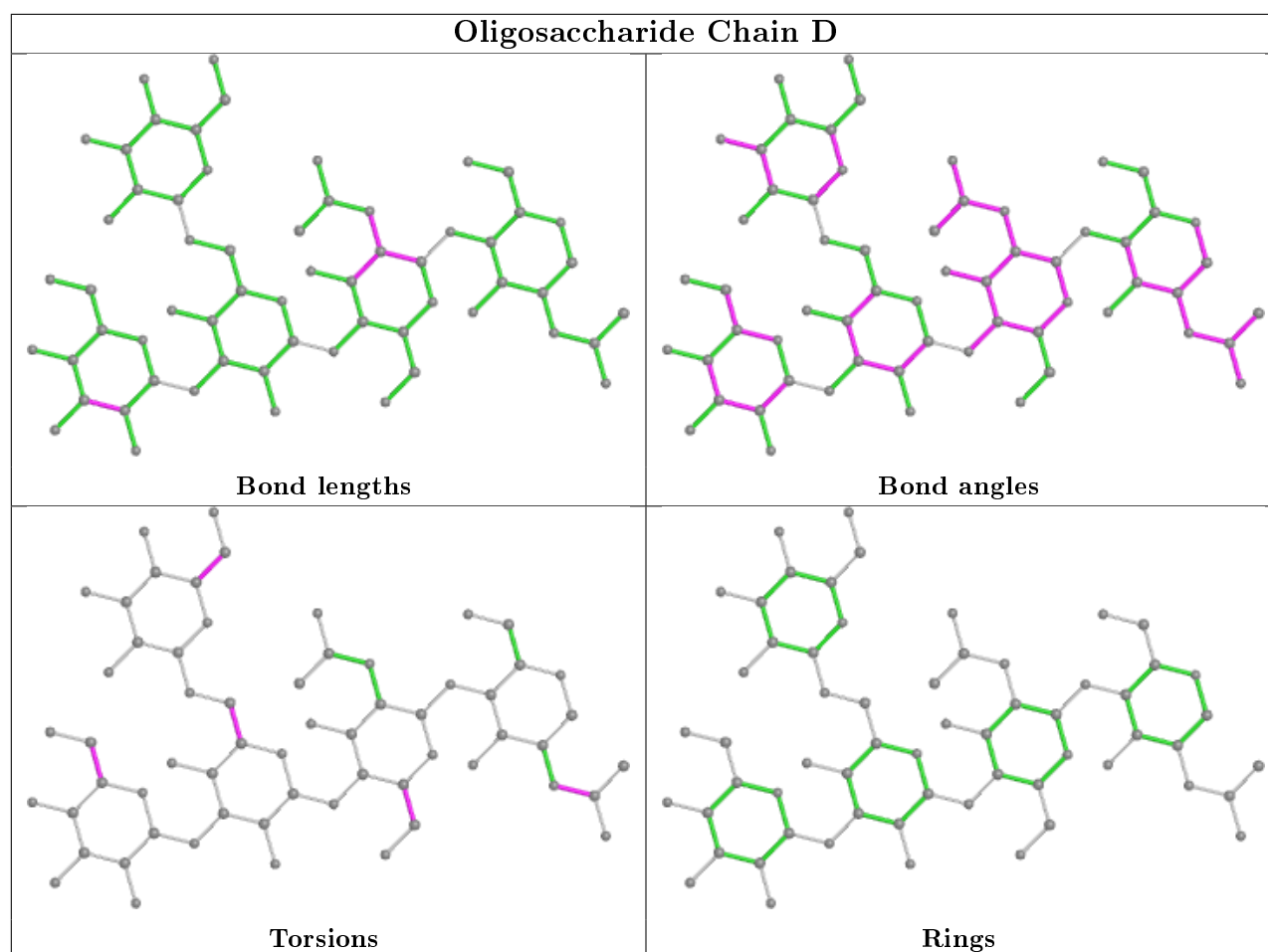
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
4	D	3	BMA	1	0
4	D	2	NAG	1	0
3	C	2	NAG	2	0
4	D	5	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	0.58	0	2,2,2	0.11	0
7	EDO	A	3333	-	3,3,3	0.49	0	2,2,2	0.27	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	B	3333	EDO	O1-C1-C2-O2
7	A	3333	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3333	EDO	2	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%)	-0.60	5 (0%) 86 79	98, 154, 230, 309	0
2	B	606/685 (88%)	-0.64	1 (0%) 95 93	99, 155, 213, 290	0
All	All	1218/1445 (84%)	-0.62	6 (0%) 91 85	98, 154, 223, 309	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	PRO	4.2
1	A	185	ALA	2.8
1	A	713	LYS	2.6
1	A	420	GLY	2.3
2	B	1802	PRO	2.2
1	A	184	LEU	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.

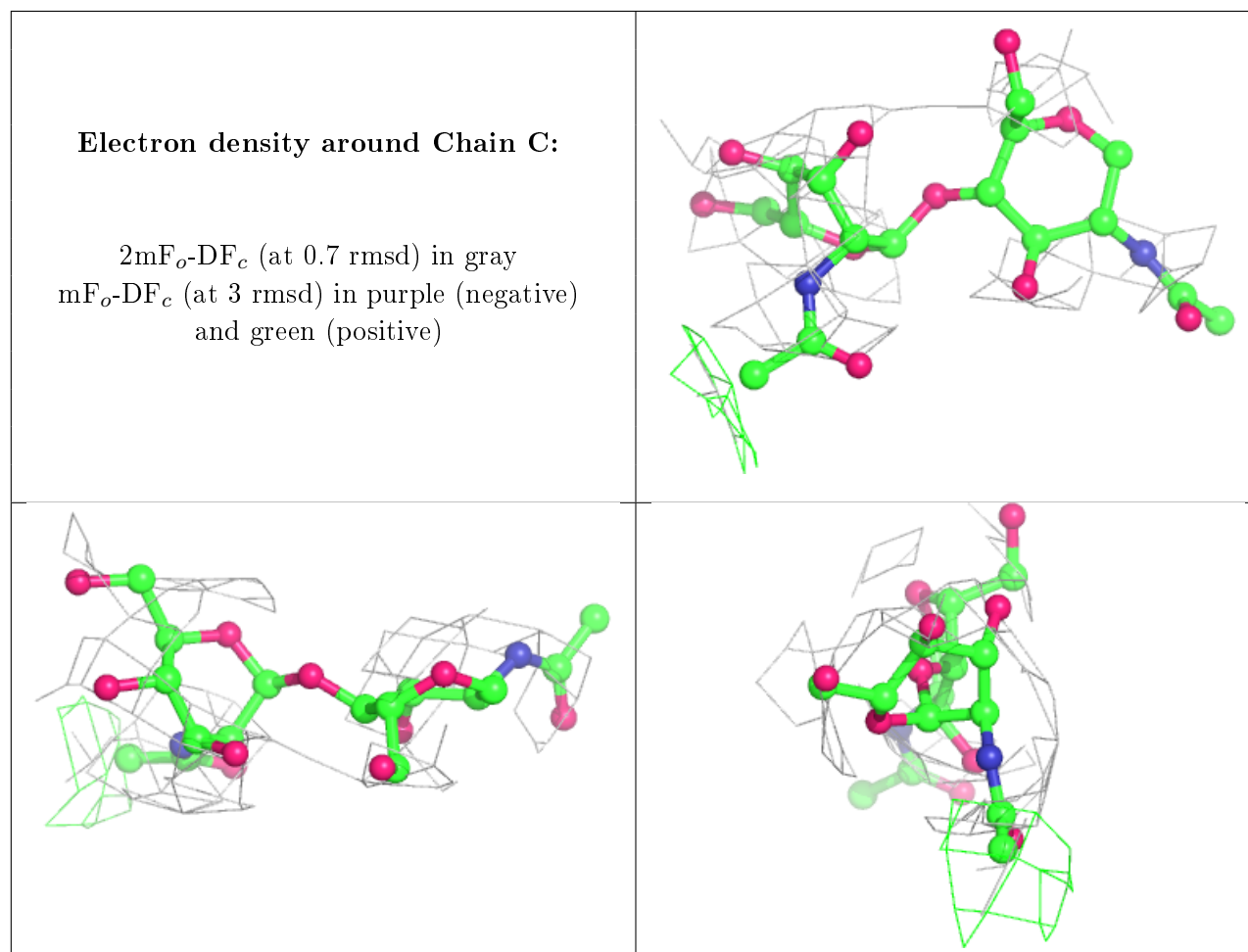
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.72	0.46	217,256,320,356	0
4	BMA	D	4	11/12	0.78	0.28	221,270,291,291	0
4	BMA	D	5	11/12	0.82	0.26	211,251,269,270	0

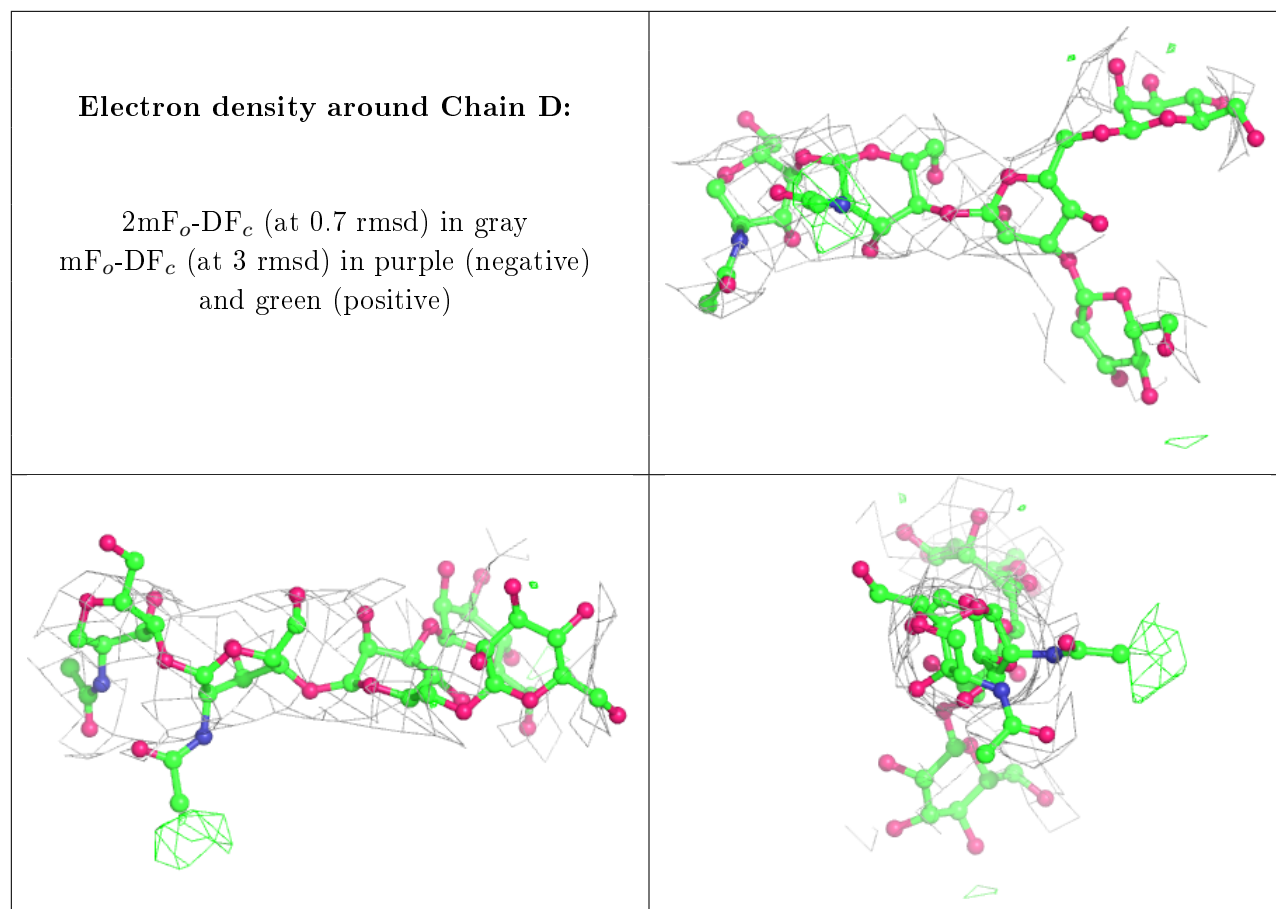
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	C	1	14/15	0.89	0.41	197,223,245,258	0
4	NAG	D	2	14/15	0.91	0.24	164,205,234,248	0
4	BMA	D	3	11/12	0.92	0.28	202,237,263,297	0
4	NAG	D	1	14/15	0.94	0.20	151,173,209,221	0

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.





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(\AA^2)	Q<0.9
7	EDO	A	3333	4/4	0.70	0.43	170,174,186,187	0
7	EDO	B	3333	4/4	0.74	0.48	129,134,141,143	0
6	CA	A	801	1/1	0.97	0.10	130,130,130,130	0
8	CU1	B	1	1/1	0.98	0.16	133,133,133,133	0
5	ZN	A	800	1/1	0.99	0.14	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.