Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 04:27 AM EDT

PDB ID	:	3CDZ
Title	:	Crystal structure of human factor VIII
Authors	:	Ngo, J.C.; Huang, M.; Roth, D.A.; Furie, B.C.; Furie, B.
Deposited on	:	2008-02-27
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

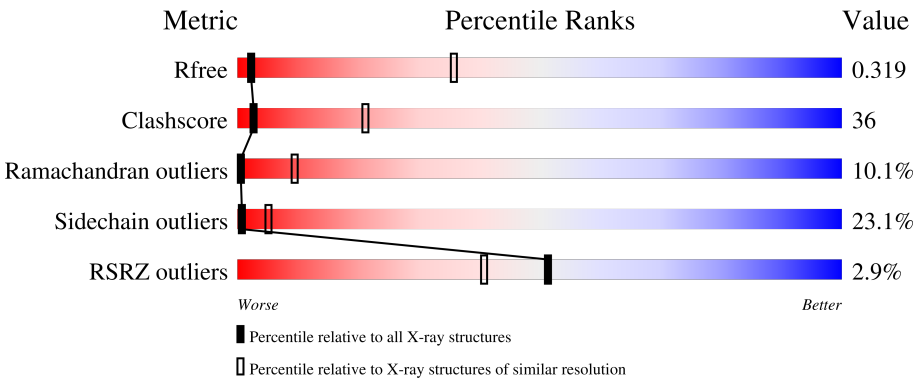
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	754	2%, 27%, 38%, 15%, •, 16%
2	B	684	3%, 36%, 41%, 14%, •, 8%
3	C	2	50%, 50%
4	D	4	75%, 25%

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
4	MAN	D	2	X	-	-	-
4	MAN	D	4	X	-	-	-
7	NAG	B	2333	X	-	-	-
7	NAG	B	2334	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10317 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coagulation factor VIII heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	630	5086	3278	855	928	25	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	SER	-	SEE REMARK 999	UNP P00451
A	742	PHE	-	SEE REMARK 999	UNP P00451
A	743	SER	-	SEE REMARK 999	UNP P00451
A	744	GLN	-	SEE REMARK 999	UNP P00451
A	745	ASN	-	SEE REMARK 999	UNP P00451
A	746	PRO	-	SEE REMARK 999	UNP P00451
A	747	PRO	-	SEE REMARK 999	UNP P00451
A	748	VAL	-	SEE REMARK 999	UNP P00451
A	749	LEU	-	SEE REMARK 999	UNP P00451
A	750	LYS	-	SEE REMARK 999	UNP P00451
A	751	ARG	-	SEE REMARK 999	UNP P00451
A	752	HIS	-	SEE REMARK 999	UNP P00451
A	753	GLN	-	SEE REMARK 999	UNP P00451
A	754	ARG	-	SEE REMARK 999	UNP P00451

- Molecule 2 is a protein called Coagulation factor VIII light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	631	5125	3288	881	924	32	0	0	0

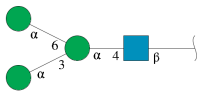
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1880	LEU	PHE	variant	UNP P00451

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	4	47	26	1	20	0	0	0

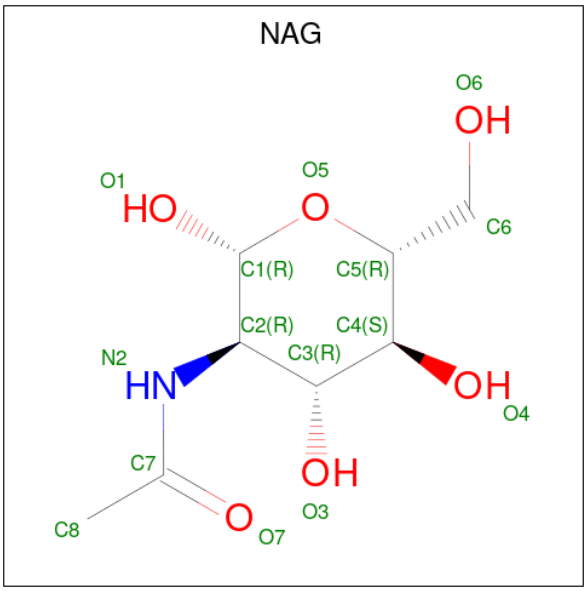
- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



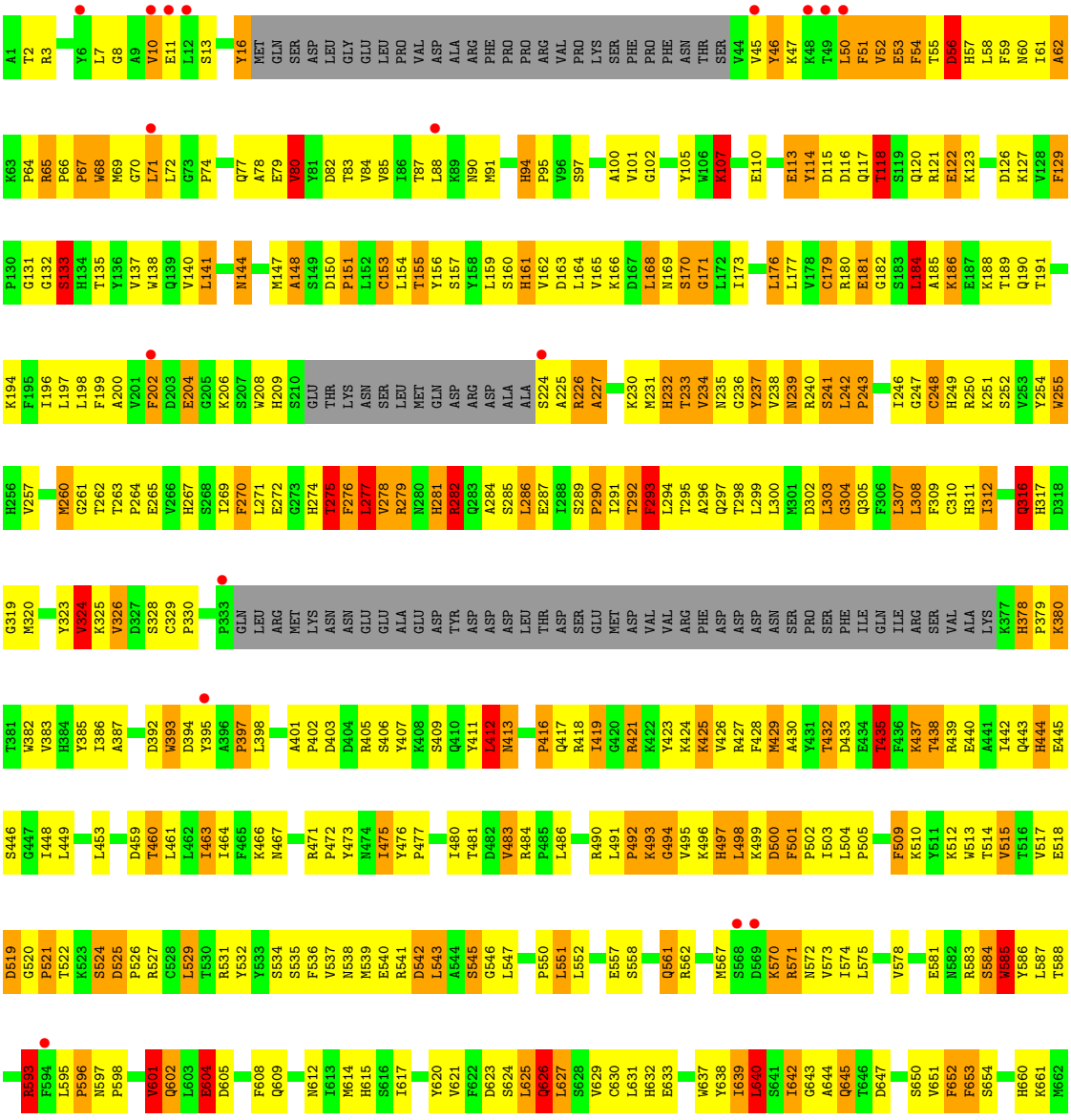
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0

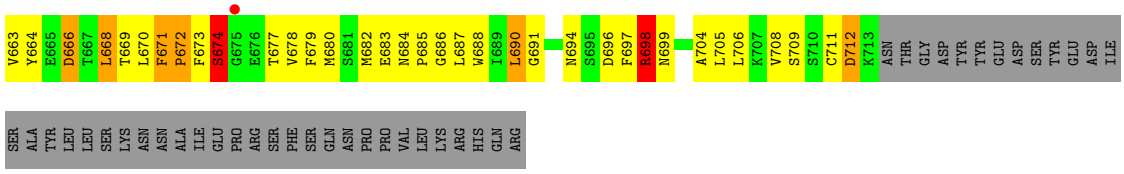
3 Residue-property plots (i)

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

- Molecule 1: Coagulation factor VIII heavy chain

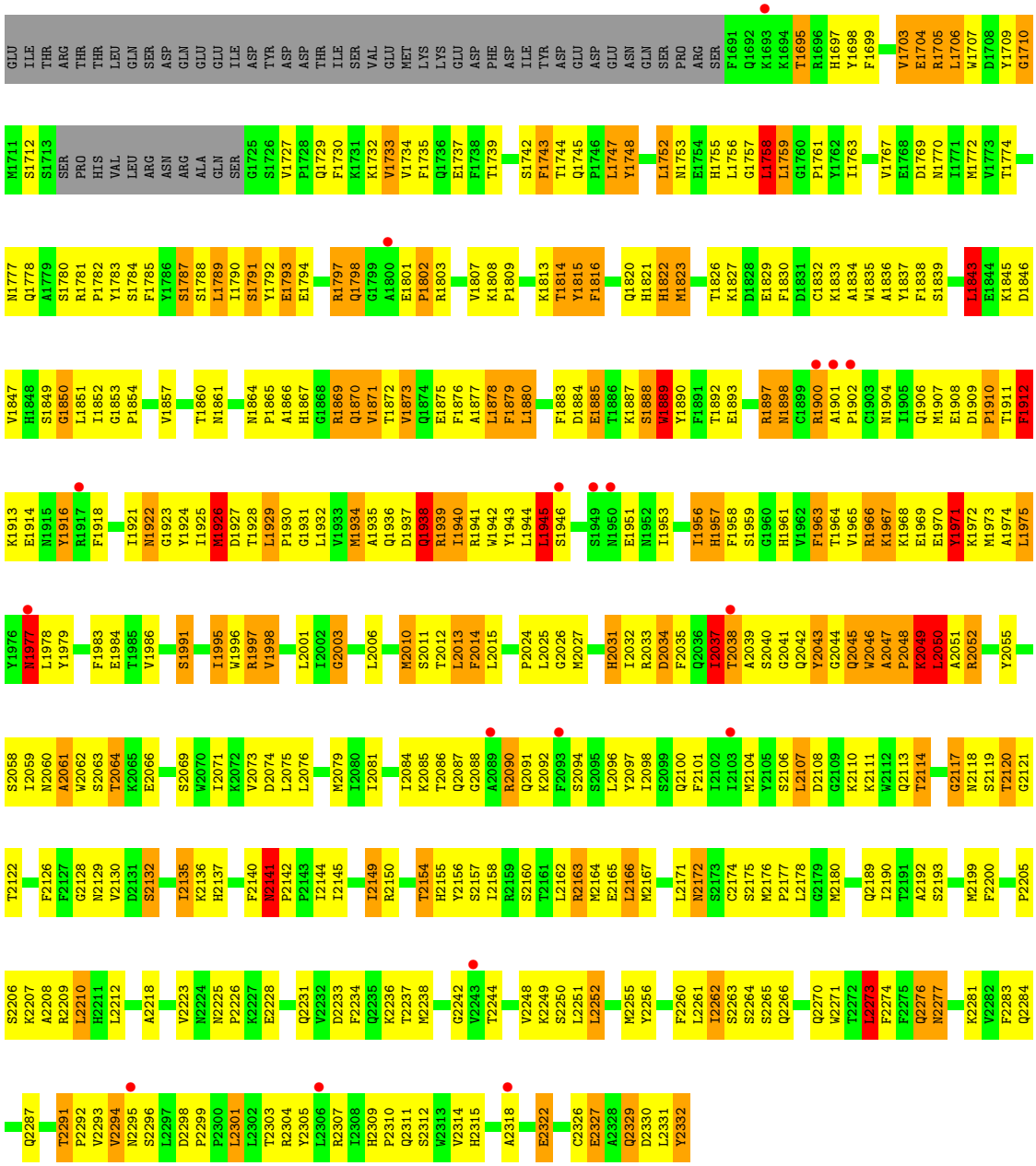
Chain A: 2% 27% 38% 15% • 16%





• Molecule 2: Coagulation factor VIII light chain

Chain B:



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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.11Å 134.11Å 349.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.98 49.66 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.98) 98.6 (49.66-3.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.256 , 0.327 0.251 , 0.319	Depositor DCC
R_{free} test set	1399 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	151.1	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 203.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10317	wwPDB-VP
Average B, all atoms (Å^2)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.74	8/5230 (0.2%)	0.94	8/7098 (0.1%)
2	B	0.62	2/5270 (0.0%)	0.77	6/7136 (0.1%)
All	All	0.68	10/10500 (0.1%)	0.86	14/14234 (0.1%)

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	7
2	B	0	6
All	All	0	13

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	ARG	CZ-NH1	13.13	1.50	1.33
2	B	1904	ASN	CG-OD1	9.72	1.45	1.24
1	A	121	ARG	NE-CZ	8.65	1.44	1.33
2	B	1904	ASN	CG-ND2	8.33	1.53	1.32
1	A	107	LYS	CG-CD	6.53	1.74	1.52
1	A	121	ARG	CZ-NH2	6.47	1.41	1.33
1	A	602	GLN	CD-NE2	6.35	1.48	1.32
1	A	122	GLU	CD-OE2	5.42	1.31	1.25
1	A	53	GLU	CB-CG	5.15	1.61	1.52
1	A	153	CYS	CB-SG	-5.06	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ARG	NE-CZ-NH2	-24.01	108.29	120.30
1	A	121	ARG	NE-CZ-NH1	23.51	132.06	120.30
2	B	1945	LEU	CA-CB-CG	7.79	133.22	115.30
1	A	277	LEU	CA-CB-CG	7.46	132.46	115.30
2	B	2050	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	121	ARG	CD-NE-CZ	-6.67	114.26	123.60
1	A	398	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	184	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	279	ARG	N-CA-C	-5.89	95.09	111.00
2	B	2049	LYS	N-CA-C	-5.43	96.35	111.00
2	B	1758	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	2273	LEU	CA-CB-CG	5.23	127.33	115.30
2	B	1971	TYR	CA-CB-CG	5.22	123.32	113.40
1	A	640	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Peptide
1	A	278	VAL	Peptide
1	A	281	HIS	Peptide
1	A	282	ARG	Peptide
1	A	293	PHE	Peptide
1	A	56	ASP	Peptide
1	A	673	PHE	Peptide
2	B	1705	ARG	Peptide
2	B	1878	LEU	Peptide
2	B	1885	GLU	Peptide
2	B	2048	PRO	Peptide
2	B	2141	ASN	Peptide
2	B	2171	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5086	0	4971	402	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5125	0	4994	354	0
3	C	28	0	25	1	0
4	D	47	0	40	2	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	B	28	0	26	0	0
All	All	10317	0	10056	737	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 36.

All (737) 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:107:LYS:CG	1:A:107:LYS:CD	1.74	1.58
1:A:378:HIS:HB3	1:A:379:PRO:CD	1.71	1.19
2:B:1963:PHE:CD2	2:B:1986:VAL:HG21	1.77	1.18
1:A:412:LEU:CB	1:A:421:ARG:HG2	1.76	1.15
1:A:572:ASN:HB3	1:A:637:TRP:CZ3	1.82	1.15
2:B:1921:ILE:N	2:B:1925:ILE:HG13	1.67	1.09
2:B:2047:ALA:HA	2:B:2062:TRP:HD1	1.10	1.09
1:A:525:ASP:HB3	1:A:526:PRO:HD2	1.33	1.09
2:B:2052:ARG:HG2	2:B:2052:ARG:HH11	1.19	1.08
2:B:1706:LEU:HD23	2:B:1730:PHE:HB3	1.13	1.07
2:B:1963:PHE:HD2	2:B:1986:VAL:CG2	1.68	1.06
1:A:572:ASN:HB3	1:A:637:TRP:HZ3	1.13	1.06
2:B:1963:PHE:HD2	2:B:1986:VAL:HG21	0.88	1.04
1:A:287:GLU:HB2	1:A:671:PHE:CE1	1.94	1.02
2:B:2047:ALA:HA	2:B:2062:TRP:CD1	1.93	1.02
1:A:501:PHE:H	1:A:502:PRO:HD3	1.21	1.01
2:B:1921:ILE:H	2:B:1925:ILE:CG1	1.72	1.00
2:B:1921:ILE:H	2:B:1925:ILE:HG13	0.84	1.00
2:B:1923:GLY:H	2:B:1925:ILE:HG12	1.27	1.00
1:A:289:SER:HB2	1:A:290:PRO:HD2	1.43	1.00
1:A:412:LEU:HB3	1:A:421:ARG:HG2	1.43	0.99
2:B:1706:LEU:HD23	2:B:1730:PHE:CB	1.91	0.99
1:A:199:PHE:CE2	1:A:269:ILE:HG12	1.98	0.98
1:A:572:ASN:CB	1:A:637:TRP:HZ3	1.75	0.98
1:A:412:LEU:HB2	1:A:421:ARG:HG2	1.42	0.97
1:A:574:ILE:HB	1:A:639:ILE:HG22	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1706:LEU:HD22	2:B:1732:LYS:H	1.31	0.95
2:B:1706:LEU:CD2	2:B:1730:PHE:HB3	1.97	0.94
1:A:294:LEU:HD21	2:B:1971:TYR:HE2	1.33	0.93
1:A:671:PHE:HB3	1:A:672:PRO:CD	1.98	0.93
1:A:277:LEU:HB2	1:A:297:GLN:HG2	1.51	0.93
2:B:1869:ARG:HE	2:B:1941:ARG:HH22	1.14	0.93
1:A:670:LEU:HD22	1:A:674:SER:HB3	1.50	0.92
1:A:378:HIS:HB3	1:A:379:PRO:HD3	1.52	0.92
1:A:378:HIS:HB3	1:A:379:PRO:HD2	1.52	0.90
2:B:1706:LEU:HD21	2:B:1732:LYS:HE3	1.54	0.89
1:A:169:ASN:HD21	1:A:262:THR:HB	1.40	0.87
2:B:2037:ILE:HG13	2:B:2040:SER:O	1.73	0.87
1:A:671:PHE:HB3	1:A:672:PRO:HD3	1.57	0.87
2:B:2037:ILE:HG12	2:B:2038:THR:N	1.90	0.86
1:A:16:TYR:HD1	1:A:16:TYR:H	1.23	0.86
1:A:232:HIS:O	1:A:232:HIS:ND1	2.09	0.86
1:A:114:TYR:OH	2:B:1997:ARG:NH1	2.08	0.85
1:A:294:LEU:HD21	2:B:1971:TYR:CE2	2.11	0.85
1:A:643:GLY:O	1:A:645:GLN:NE2	2.09	0.85
2:B:1798:GLN:CG	2:B:1802:PRO:HD2	2.06	0.85
1:A:100:ALA:HB2	1:A:138:TRP:CZ2	2.12	0.85
2:B:2052:ARG:HH11	2:B:2052:ARG:CG	1.88	0.85
2:B:1756:LEU:O	2:B:1759:LEU:HD12	1.77	0.85
2:B:1849:SER:OG	2:B:1888:SER:HB3	1.77	0.85
2:B:1739:THR:HB	2:B:1745:GLN:HB2	1.59	0.85
1:A:287:GLU:HB2	1:A:671:PHE:HE1	1.39	0.85
1:A:626:GLN:HG2	1:A:627:LEU:H	1.39	0.85
1:A:276:PHE:CE1	1:A:518:GLU:O	2.31	0.84
2:B:2218:ALA:HB3	2:B:2248:VAL:HG11	1.59	0.84
2:B:1877:ALA:O	2:B:1878:LEU:HD12	1.78	0.84
1:A:271:LEU:HD23	1:A:308:LEU:HD22	1.61	0.83
1:A:118:THR:HG22	1:A:122:GLU:HB3	1.60	0.83
2:B:2047:ALA:HB1	2:B:2048:PRO:HD2	1.60	0.83
2:B:1789:LEU:HB2	2:B:1823:MET:HG3	1.60	0.82
1:A:132:GLY:O	1:A:133:SER:HB2	1.80	0.81
2:B:1929:LEU:H	2:B:2012:THR:HG23	1.46	0.81
2:B:2234:PHE:CD2	2:B:2238:MET:HG3	2.16	0.81
2:B:1759:LEU:HD23	2:B:1852:ILE:HG22	1.60	0.81
1:A:287:GLU:HB2	1:A:671:PHE:CD1	2.15	0.81
1:A:16:TYR:HD1	1:A:16:TYR:N	1.75	0.80
1:A:630:CYS:HB2	1:A:709:SER:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1885:GLU:HG3	2:B:1914:GLU:OE2	1.82	0.80
1:A:186:LYS:O	1:A:190:GLN:HB2	1.81	0.80
1:A:270:PHE:O	1:A:308:LEU:HD13	1.82	0.80
1:A:87:THR:HG22	1:A:135:THR:HG23	1.63	0.79
1:A:153:CYS:HA	1:A:179:CYS:HB3	1.62	0.79
2:B:2314:VAL:HG13	2:B:2315:HIS:H	1.45	0.79
2:B:1921:ILE:O	2:B:1922:ASN:HB2	1.82	0.79
1:A:378:HIS:CB	1:A:379:PRO:CD	2.58	0.79
2:B:1781:ARG:HH22	2:B:1888:SER:HA	1.48	0.79
1:A:557:GLU:HA	1:A:561:GLN:HG3	1.64	0.78
2:B:1912:PHE:O	2:B:1916:TYR:HB2	1.84	0.78
1:A:525:ASP:HB3	1:A:526:PRO:CD	2.13	0.77
2:B:1798:GLN:HG2	2:B:1802:PRO:HD2	1.66	0.77
1:A:429:MET:HG3	1:A:439:ARG:HH22	1.48	0.76
1:A:660:HIS:O	1:A:661:LYS:HG2	1.84	0.76
2:B:1923:GLY:H	2:B:1925:ILE:CG1	1.98	0.76
2:B:2314:VAL:HG13	2:B:2315:HIS:N	2.01	0.76
1:A:164:LEU:HD22	2:B:2003:GLY:HA2	1.67	0.76
2:B:1706:LEU:HD13	2:B:1732:LYS:HB2	1.66	0.76
1:A:492:PRO:O	1:A:494:GLY:N	2.18	0.75
1:A:246:ILE:HD12	1:A:247:GLY:H	1.52	0.75
1:A:107:LYS:CD	1:A:107:LYS:CB	2.65	0.75
2:B:2120:THR:HG23	2:B:2121:GLY:H	1.51	0.75
1:A:471:ARG:HG3	1:A:585:TRP:CE3	2.22	0.74
2:B:1984:GLU:OE1	2:B:1984:GLU:HA	1.87	0.74
2:B:1834:ALA:HB2	2:B:1943:TYR:HD2	1.52	0.74
2:B:2037:ILE:HG12	2:B:2038:THR:H	1.52	0.74
2:B:1706:LEU:CD1	2:B:1732:LYS:HB2	2.19	0.73
2:B:2118:ASN:ND2	2:B:2141:ASN:HB3	2.04	0.73
1:A:501:PHE:N	1:A:502:PRO:HD3	2.01	0.73
2:B:1798:GLN:HG3	2:B:1802:PRO:HD2	1.71	0.73
2:B:1921:ILE:HB	2:B:1925:ILE:HD12	1.70	0.73
2:B:1789:LEU:HB2	2:B:1823:MET:CG	2.18	0.73
1:A:412:LEU:HB2	1:A:421:ARG:CG	2.18	0.73
1:A:7:LEU:CD1	1:A:74:PRO:HG2	2.19	0.72
2:B:2218:ALA:CB	2:B:2248:VAL:HG11	2.19	0.72
1:A:277:LEU:HD23	1:A:297:GLN:HE21	1.54	0.72
2:B:2052:ARG:HG2	2:B:2052:ARG:NH1	1.98	0.72
2:B:2094:SER:HB3	2:B:2158:ILE:HD13	1.71	0.72
1:A:428:PHE:HE2	1:A:475:ILE:CG2	2.03	0.71
1:A:574:ILE:HB	1:A:639:ILE:CG2	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1864:ASN:HD22	2:B:1865:PRO:HD2	1.56	0.71
2:B:1737:GLU:HB2	2:B:1761:PRO:HG3	1.71	0.71
1:A:386:ILE:HD12	1:A:463:ILE:HD11	1.72	0.71
1:A:393:TRP:HA	1:A:393:TRP:CE3	2.25	0.71
2:B:1923:GLY:N	2:B:1925:ILE:HG12	2.05	0.71
2:B:1869:ARG:NE	2:B:1941:ARG:HH22	1.87	0.71
1:A:54:PHE:H	1:A:54:PHE:HD1	1.37	0.70
1:A:413:ASN:HB3	1:A:595:LEU:HD23	1.73	0.70
2:B:1959:SER:HB3	2:B:1997:ARG:HH22	1.57	0.70
2:B:2035:PHE:CD2	2:B:2074:ASP:HB2	2.27	0.70
1:A:378:HIS:CB	1:A:379:PRO:HD3	2.22	0.70
1:A:50:LEU:HD21	1:A:71:LEU:HA	1.73	0.70
2:B:1996:TRP:HB2	2:B:2014:PHE:CE2	2.26	0.70
1:A:464:ILE:HG23	1:A:510:LYS:HG2	1.73	0.70
2:B:2199:MET:HG3	2:B:2200:PHE:N	2.06	0.70
1:A:527:ARG:HH22	1:A:562:ARG:HB3	1.56	0.69
2:B:1759:LEU:HG	2:B:1879:PHE:CD2	2.27	0.69
1:A:107:LYS:CG	1:A:107:LYS:CE	2.68	0.69
1:A:386:ILE:HA	1:A:430:ALA:HA	1.74	0.69
1:A:501:PHE:H	1:A:502:PRO:CD	2.02	0.69
2:B:2024:PRO:HA	2:B:2167:MET:HE2	1.74	0.69
2:B:1834:ALA:HB2	2:B:1943:TYR:CD2	2.27	0.69
1:A:626:GLN:HB2	1:A:705:LEU:O	1.93	0.69
1:A:497:HIS:CE1	1:A:499:LYS:HG2	2.27	0.69
2:B:2225:ASN:O	2:B:2228:GLU:HB2	1.92	0.68
1:A:480:ILE:HG12	1:A:515:VAL:HG13	1.76	0.68
1:A:16:TYR:N	1:A:16:TYR:CD1	2.49	0.68
1:A:572:ASN:HB3	1:A:637:TRP:CE3	2.27	0.68
1:A:147:MET:HG2	2:B:1972:LYS:HD3	1.76	0.68
2:B:2192:ALA:HB2	2:B:2205:PRO:HB3	1.75	0.68
1:A:8:GLY:O	1:A:52:VAL:HG23	1.94	0.67
2:B:2025:LEU:HD12	2:B:2166:LEU:HB3	1.76	0.67
2:B:2094:SER:HB3	2:B:2158:ILE:CD1	2.24	0.67
1:A:271:LEU:CD2	1:A:308:LEU:HD22	2.24	0.67
2:B:1921:ILE:O	2:B:1921:ILE:HG22	1.93	0.67
2:B:2218:ALA:CB	2:B:2248:VAL:CG1	2.73	0.67
1:A:310:CYS:SG	5:A:757:CU:CU	1.84	0.67
1:A:630:CYS:O	1:A:633:GLU:HB2	1.95	0.66
2:B:1706:LEU:HG	2:B:1707:TRP:HB2	1.77	0.66
1:A:626:GLN:HG2	1:A:627:LEU:N	2.08	0.66
1:A:626:GLN:CG	1:A:627:LEU:H	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HA	1:A:230:LYS:HZ2	1.61	0.65
1:A:694:ASN:O	1:A:698:ARG:HG2	1.97	0.65
1:A:275:THR:HG21	1:A:286:LEU:HD22	1.77	0.65
1:A:453:LEU:HB3	1:A:551:LEU:HD23	1.77	0.65
1:A:535:SER:HB3	1:A:547:LEU:HD13	1.77	0.65
2:B:2118:ASN:H	2:B:2142:PRO:HD3	1.61	0.65
1:A:53:GLU:OE2	1:A:65:ARG:HG2	1.96	0.64
2:B:1781:ARG:NH2	2:B:1888:SER:HA	2.13	0.64
2:B:2261:LEU:HB2	2:B:2309:HIS:HB2	1.78	0.64
1:A:55:THR:HG23	1:A:60:ASN:HD21	1.61	0.64
1:A:393:TRP:HA	1:A:393:TRP:HE3	1.63	0.63
1:A:159:LEU:HD12	1:A:160:SER:H	1.61	0.63
1:A:279:ARG:C	1:A:281:HIS:H	2.02	0.63
2:B:1695:THR:HB	2:B:1770:ASN:HD22	1.62	0.63
2:B:2210:LEU:HD11	2:B:2244:THR:HG22	1.79	0.63
1:A:156:TYR:HA	1:A:293:PHE:CE2	2.34	0.63
1:A:277:LEU:HB3	1:A:296:ALA:HA	1.80	0.63
2:B:2298:ASP:HB3	2:B:2299:PRO:HD3	1.80	0.63
2:B:2037:ILE:HG22	2:B:2071:ILE:HA	1.81	0.63
1:A:271:LEU:HD23	1:A:308:LEU:CD2	2.28	0.62
2:B:1997:ARG:HB2	2:B:2013:LEU:HA	1.80	0.62
2:B:1997:ARG:O	2:B:1997:ARG:NH2	2.32	0.62
1:A:275:THR:HA	1:A:298:THR:CG2	2.29	0.62
2:B:2145:ILE:O	2:B:2145:ILE:HD12	1.99	0.62
2:B:1782:PRO:HG3	2:B:1809:PRO:HD3	1.80	0.62
1:A:299:LEU:C	1:A:300:LEU:HG	2.20	0.62
1:A:651:VAL:HG22	1:A:668:LEU:HB3	1.80	0.62
2:B:1914:GLU:HG3	2:B:1918:PHE:CD2	2.34	0.62
1:A:540:GLU:C	1:A:542:ASP:N	2.52	0.62
2:B:1964:THR:O	2:B:1986:VAL:HG23	2.00	0.62
1:A:100:ALA:HB2	1:A:138:TRP:CH2	2.34	0.61
1:A:293:PHE:N	1:A:293:PHE:CD1	2.67	0.61
1:A:3:ARG:NH1	1:A:78:ALA:HA	2.15	0.61
1:A:249:HIS:NE2	1:A:250:ARG:HG2	2.15	0.61
1:A:638:TYR:CD1	1:A:677:THR:HG23	2.35	0.61
1:A:85:VAL:HG12	1:A:85:VAL:O	2.01	0.61
2:B:2027:MET:HG3	2:B:2165:GLU:HA	1.83	0.61
1:A:525:ASP:CB	1:A:526:PRO:HD2	2.21	0.61
2:B:1732:LYS:NZ	2:B:1918:PHE:CE1	2.67	0.61
1:A:275:THR:O	1:A:275:THR:HG23	2.00	0.61
2:B:1704:GLU:HB3	2:B:1732:LYS:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:N	1:A:129:PHE:CD2	2.68	0.61
1:A:141:LEU:N	1:A:144:ASN:HD21	1.97	0.61
1:A:234:VAL:C	1:A:236:GLY:H	2.03	0.61
2:B:1752:LEU:HD12	2:B:2118:ASN:HA	1.83	0.61
2:B:1833:LYS:HG2	2:B:1966:ARG:HH22	1.65	0.61
2:B:2048:PRO:O	2:B:2049:LYS:HB2	2.00	0.61
1:A:267:HIS:ND1	1:A:310:CYS:SG	2.74	0.61
1:A:246:ILE:CD1	1:A:247:GLY:H	2.14	0.61
1:A:246:ILE:HG13	1:A:247:GLY:N	2.14	0.60
1:A:275:THR:OG1	1:A:286:LEU:HD21	2.01	0.60
1:A:491:LEU:O	1:A:493:LYS:N	2.34	0.60
2:B:1789:LEU:HD22	2:B:1791:SER:OG	2.00	0.60
2:B:2193:SER:HB3	2:B:2228:GLU:OE1	2.01	0.60
2:B:2031:HIS:HB2	2:B:2034:ASP:HB2	1.84	0.60
1:A:246:ILE:CD1	1:A:326:VAL:H	2.14	0.60
2:B:1890:TYR:HA	2:B:1893:GLU:OE1	2.02	0.60
2:B:2066:GLU:HB3	2:B:2069:SER:OG	2.01	0.60
1:A:572:ASN:CG	1:A:637:TRP:HZ3	2.04	0.60
2:B:2096:LEU:HB3	2:B:2158:ILE:HD12	1.84	0.60
1:A:282:ARG:HD2	1:A:522:THR:HG21	1.83	0.60
1:A:150:ASP:HB2	1:A:151:PRO:HD2	1.84	0.60
1:A:274:HIS:CE1	1:A:519:ASP:HB3	2.37	0.60
2:B:2242:GLY:HA3	2:B:2296:SER:HA	1.84	0.60
1:A:393:TRP:HE1	1:A:448:ILE:HB	1.67	0.60
1:A:575:LEU:HD11	1:A:642:ILE:HG22	1.83	0.60
1:A:286:LEU:HD22	1:A:286:LEU:H	1.65	0.60
2:B:1787:SER:HB2	2:B:1836:ALA:O	2.00	0.60
2:B:1888:SER:O	2:B:1890:TYR:N	2.35	0.60
2:B:2281:LYS:HG2	2:B:2283:PHE:CZ	2.37	0.60
1:A:199:PHE:HE2	1:A:269:ILE:HG12	1.61	0.59
1:A:234:VAL:O	1:A:236:GLY:N	2.35	0.59
1:A:666:ASP:HB3	2:B:1835:TRP:HZ3	1.66	0.59
2:B:2052:ARG:CG	2:B:2052:ARG:NH1	2.57	0.59
1:A:430:ALA:O	1:A:440:GLU:HB2	2.03	0.59
2:B:2149:ILE:N	2:B:2149:ILE:HD12	2.18	0.59
1:A:477:PRO:HG3	1:A:513:TRP:CE2	2.37	0.59
1:A:54:PHE:HA	1:A:62:ALA:HB3	1.85	0.59
2:B:2052:ARG:O	2:B:2163:ARG:HB2	2.02	0.59
1:A:238:VAL:O	1:A:240:ARG:N	2.36	0.59
1:A:289:SER:HB2	1:A:290:PRO:CD	2.27	0.58
2:B:1787:SER:OG	2:B:1788:SER:N	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1879:PHE:CD1	2:B:1879:PHE:N	2.72	0.58
1:A:169:ASN:ND2	1:A:262:THR:HB	2.16	0.58
2:B:2047:ALA:HB1	2:B:2048:PRO:CD	2.31	0.58
1:A:230:LYS:HZ1	1:A:231:MET:H	1.51	0.58
1:A:581:GLU:HB2	1:A:612:ASN:HB3	1.86	0.58
1:A:240:ARG:O	1:A:242:LEU:HD13	2.04	0.58
1:A:498:LEU:HD12	1:A:498:LEU:H	1.69	0.58
1:A:289:SER:CB	1:A:290:PRO:HD2	2.27	0.58
1:A:640:LEU:HA	1:A:674:SER:O	2.04	0.58
2:B:1695:THR:HA	2:B:1770:ASN:CB	2.34	0.58
2:B:2074:ASP:O	2:B:2076:LEU:HD22	2.03	0.58
1:A:471:ARG:HD2	1:A:585:TRP:CZ3	2.39	0.57
2:B:2037:ILE:HG21	2:B:2040:SER:O	2.04	0.57
1:A:393:TRP:HE3	1:A:394:ASP:H	1.52	0.57
2:B:2051:ALA:HA	2:B:2061:ALA:HA	1.86	0.57
1:A:572:ASN:CB	1:A:637:TRP:CZ3	2.62	0.57
2:B:1785:PHE:CZ	2:B:1815:TYR:HB2	2.40	0.57
2:B:1959:SER:HB3	2:B:1997:ARG:NH2	2.19	0.57
2:B:1937:ASP:O	2:B:1938:GLN:C	2.42	0.57
1:A:141:LEU:H	1:A:144:ASN:HD21	1.51	0.57
1:A:276:PHE:HE1	1:A:518:GLU:O	1.86	0.57
1:A:498:LEU:C	1:A:500:ASP:H	2.08	0.57
2:B:1789:LEU:HD12	2:B:1823:MET:HG3	1.87	0.57
2:B:1940:ILE:HG13	2:B:1940:ILE:O	2.04	0.57
1:A:626:GLN:CG	1:A:627:LEU:N	2.64	0.57
2:B:1829:GLU:HA	2:B:1966:ARG:HG3	1.87	0.57
1:A:428:PHE:HE1	1:A:547:LEU:HB3	1.69	0.56
1:A:638:TYR:HD1	1:A:677:THR:HG23	1.69	0.56
2:B:1937:ASP:O	2:B:1939:ARG:N	2.38	0.56
1:A:246:ILE:CG1	1:A:247:GLY:N	2.68	0.56
1:A:299:LEU:O	1:A:300:LEU:HG	2.06	0.56
2:B:1910:PRO:HA	2:B:1912:PHE:CE2	2.40	0.56
2:B:2033:ARG:HG2	2:B:2049:LYS:HA	1.87	0.56
2:B:2256:TYR:H	2:B:2314:VAL:HG12	1.70	0.56
2:B:2043:TYR:O	2:B:2045:GLN:N	2.39	0.56
2:B:1883:PHE:O	2:B:1914:GLU:HB3	2.06	0.56
1:A:270:PHE:O	1:A:308:LEU:CD1	2.54	0.56
1:A:448:ILE:HD11	1:A:546:GLY:HA2	1.88	0.56
1:A:496:LYS:O	1:A:497:HIS:HB3	2.05	0.56
1:A:70:GLY:H	1:A:72:LEU:HD12	1.71	0.56
1:A:663:VAL:HG12	1:A:664:TYR:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1789:LEU:CB	2:B:1823:MET:HG3	2.34	0.56
2:B:2266:GLN:HE22	2:B:2303:THR:HA	1.71	0.56
1:A:538:ASN:O	1:A:542:ASP:HB2	2.06	0.55
1:A:185:ALA:HA	1:A:188:LYS:HD2	1.87	0.55
2:B:2264:SER:HB3	2:B:2301:LEU:HD11	1.87	0.55
1:A:232:HIS:O	1:A:232:HIS:CG	2.59	0.55
1:A:246:ILE:HG12	1:A:326:VAL:N	2.21	0.55
2:B:1735:PHE:CE2	2:B:1851:LEU:HB3	2.41	0.55
2:B:1889:TRP:O	2:B:1892:THR:HG22	2.05	0.55
1:A:7:LEU:HD13	1:A:74:PRO:HG2	1.88	0.55
1:A:416:PRO:HB2	1:A:596:PRO:HG2	1.88	0.55
1:A:393:TRP:CH2	1:A:620:TYR:HE1	2.24	0.55
1:A:471:ARG:CG	1:A:585:TRP:CE3	2.90	0.55
1:A:605:ASP:HB3	1:A:608:PHE:HB3	1.88	0.55
2:B:2045:GLN:O	2:B:2045:GLN:HG2	2.07	0.55
1:A:232:HIS:CE1	1:A:267:HIS:HE1	2.24	0.55
1:A:278:VAL:N	1:A:279:ARG:O	2.36	0.55
2:B:2314:VAL:CG1	2:B:2315:HIS:H	2.15	0.55
2:B:1901:ALA:N	2:B:1902:PRO:CD	2.70	0.55
1:A:540:GLU:C	1:A:542:ASP:H	2.10	0.55
1:A:385:TYR:CE2	1:A:464:ILE:HD12	2.42	0.54
2:B:1833:LYS:HD3	2:B:1834:ALA:H	1.72	0.54
2:B:1963:PHE:N	2:B:1963:PHE:CD1	2.74	0.54
2:B:1733:VAL:HG22	2:B:1889:TRP:CZ2	2.42	0.54
2:B:1864:ASN:HB3	2:B:1866:ALA:H	1.72	0.54
2:B:2250:SER:C	2:B:2252:LEU:H	2.09	0.54
1:A:97:SER:HB3	1:A:162:VAL:HG23	1.89	0.54
2:B:1885:GLU:CG	2:B:1914:GLU:OE2	2.53	0.54
2:B:2097:TYR:HB2	2:B:2129:ASN:HD22	1.72	0.54
1:A:275:THR:HA	1:A:298:THR:HG23	1.89	0.54
1:A:276:PHE:CD2	1:A:282:ARG:HB3	2.42	0.54
2:B:2314:VAL:CG1	2:B:2315:HIS:N	2.70	0.54
1:A:380:LYS:N	1:A:459:ASP:OD2	2.41	0.54
2:B:2051:ALA:O	2:B:2163:ARG:HA	2.07	0.54
1:A:155:THR:O	1:A:156:TYR:CD2	2.61	0.54
1:A:156:TYR:HA	1:A:293:PHE:CD2	2.43	0.54
1:A:406:SER:H	1:A:409:SER:HB2	1.73	0.54
2:B:1932:LEU:HB3	2:B:2014:PHE:HB2	1.90	0.54
2:B:2304:ARG:HH11	2:B:2331:LEU:HD11	1.73	0.54
2:B:1963:PHE:CD2	2:B:1986:VAL:CG2	2.61	0.54
1:A:64:PRO:O	1:A:66:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TYR:HB3	1:A:421:ARG:HD3	1.89	0.53
1:A:230:LYS:NZ	1:A:231:MET:H	2.06	0.53
1:A:538:ASN:CG	1:A:541:ARG:HB3	2.28	0.53
2:B:1934:MET:HG3	2:B:1940:ILE:HG21	1.89	0.53
2:B:2060:ASN:O	2:B:2061:ALA:CB	2.56	0.53
1:A:395:TYR:CE2	1:A:614:MET:HG3	2.43	0.53
1:A:110:GLU:OE2	2:B:1997:ARG:NH1	2.40	0.53
1:A:412:LEU:HA	1:A:423:TYR:OH	2.09	0.53
1:A:433:ASP:OD2	1:A:433:ASP:N	2.39	0.53
1:A:94:HIS:HD2	1:A:95:PRO:HD2	1.73	0.53
1:A:387:ALA:HA	1:A:466:LYS:O	2.08	0.53
1:A:671:PHE:CB	1:A:672:PRO:HD3	2.35	0.53
1:A:687:LEU:HD23	2:B:1801:GLU:O	2.09	0.53
2:B:2265:SER:HB3	2:B:2305:TYR:HB2	1.91	0.53
1:A:401:ALA:N	1:A:402:PRO:HD3	2.24	0.53
1:A:472:PRO:HB3	1:A:504:LEU:HA	1.90	0.53
2:B:1966:ARG:HA	2:B:1969:GLU:O	2.08	0.53
2:B:1789:LEU:HD21	2:B:1822:HIS:HD2	1.74	0.53
2:B:2042:GLN:HA	2:B:2046:TRP:CD1	2.44	0.53
2:B:2274:PHE:CZ	2:B:2299:PRO:HD2	2.44	0.52
1:A:461:LEU:HB2	1:A:513:TRP:HB2	1.91	0.52
2:B:1870:GLN:C	2:B:1873:VAL:HG23	2.30	0.52
2:B:1913:LYS:HA	2:B:1916:TYR:HB2	1.92	0.52
2:B:2180:MET:HG3	2:B:2322:GLU:HA	1.91	0.52
1:A:226:ARG:O	1:A:227:ALA:HB2	2.09	0.52
1:A:292:THR:C	1:A:293:PHE:HD1	2.11	0.52
1:A:584:SER:C	1:A:586:TYR:H	2.13	0.52
2:B:1838:PHE:HE2	2:B:1843:LEU:HB3	1.73	0.52
1:A:176:LEU:O	1:A:176:LEU:HG	2.08	0.52
1:A:686:GLY:HA3	2:B:1803:ARG:HD2	1.90	0.52
2:B:1924:TYR:C	2:B:1925:ILE:HD13	2.30	0.52
2:B:2060:ASN:O	2:B:2061:ALA:HB3	2.09	0.52
1:A:521:PRO:C	1:A:522:THR:HG23	2.30	0.52
1:A:578:VAL:H	1:A:644:ALA:HB2	1.75	0.52
2:B:1909:ASP:O	2:B:1911:THR:N	2.43	0.52
2:B:2331:LEU:HB3	2:B:2332:TYR:CD2	2.45	0.52
1:A:312:ILE:O	1:A:316:GLN:HB2	2.09	0.52
1:A:46:TYR:H	1:A:47:LYS:NZ	2.08	0.52
1:A:501:PHE:N	1:A:502:PRO:CD	2.66	0.52
1:A:578:VAL:HG22	1:A:615:HIS:HA	1.92	0.52
2:B:1784:SER:O	2:B:1839:SER:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1845:LYS:HD3	2:B:1888:SER:H	1.74	0.52
1:A:234:VAL:O	1:A:237:TYR:N	2.33	0.52
1:A:237:TYR:CE1	1:A:243:PRO:HA	2.45	0.52
1:A:472:PRO:O	1:A:537:VAL:HG11	2.10	0.52
1:A:467:ASN:HD21	1:A:472:PRO:HA	1.75	0.52
2:B:2189:GLN:HG2	2:B:2233:ASP:O	2.10	0.52
1:A:77:GLN:HG2	1:A:177:LEU:HB2	1.91	0.51
2:B:1789:LEU:HD12	2:B:1823:MET:HB2	1.92	0.51
2:B:2231:GLN:OE1	2:B:2271:TRP:HH2	1.94	0.51
1:A:147:MET:O	1:A:148:ALA:C	2.49	0.51
1:A:428:PHE:CE2	1:A:475:ILE:CG2	2.91	0.51
2:B:1873:VAL:HG12	2:B:1875:GLU:HG3	1.91	0.51
1:A:260:MET:HG3	1:A:261:GLY:H	1.75	0.51
1:A:432:THR:OG1	1:A:438:THR:HB	2.10	0.51
1:A:317:HIS:NE2	3:C:1:NAG:O3	2.40	0.51
2:B:2274:PHE:HZ	2:B:2299:PRO:HD2	1.74	0.51
2:B:1739:THR:HG21	2:B:1745:GLN:CG	2.41	0.51
2:B:1782:PRO:HB3	2:B:1808:LYS:HA	1.92	0.51
1:A:246:ILE:CD1	1:A:326:VAL:N	2.74	0.51
1:A:671:PHE:N	1:A:674:SER:OG	2.42	0.51
2:B:1929:LEU:HD22	2:B:2012:THR:HG21	1.93	0.51
2:B:2037:ILE:CG1	2:B:2038:THR:H	2.23	0.51
1:A:428:PHE:HE2	1:A:475:ILE:HG22	1.75	0.50
1:A:540:GLU:HA	1:A:543:LEU:HB3	1.92	0.50
1:A:525:ASP:CB	1:A:526:PRO:CD	2.84	0.50
1:A:80:VAL:CG2	1:A:181:GLU:HG3	2.41	0.50
1:A:166:LYS:O	1:A:170:SER:HB2	2.10	0.50
1:A:170:SER:OG	1:A:208:TRP:HB3	2.11	0.50
2:B:1695:THR:HA	2:B:1770:ASN:HB3	1.92	0.50
2:B:1759:LEU:C	2:B:1759:LEU:HD13	2.32	0.50
2:B:2101:PHE:O	2:B:2126:PHE:HB2	2.12	0.50
1:A:263:THR:HG23	1:A:265:GLU:HB2	1.93	0.50
2:B:1789:LEU:CD2	2:B:1822:HIS:HD2	2.25	0.50
2:B:1793:GLU:HG3	2:B:1794:GLU:HG3	1.92	0.50
2:B:1734:VAL:HA	2:B:1850:GLY:O	2.12	0.50
2:B:1897:ARG:O	2:B:1898:ASN:HB2	2.12	0.50
1:A:316:GLN:O	1:A:319:GLY:N	2.44	0.50
1:A:527:ARG:NH2	1:A:562:ARG:HB3	2.25	0.50
1:A:249:HIS:CD2	1:A:250:ARG:HG2	2.46	0.50
1:A:537:VAL:HG12	1:A:542:ASP:OD2	2.12	0.50
2:B:1706:LEU:O	2:B:1758:LEU:HD21	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2026:GLY:O	2:B:2031:HIS:NE2	2.45	0.50
1:A:202:PHE:CD1	1:A:202:PHE:N	2.79	0.50
1:A:652:PHE:O	1:A:653:PHE:HB2	2.12	0.50
2:B:2108:ASP:OD2	2:B:2108:ASP:N	2.43	0.50
2:B:2263:SER:HA	2:B:2273:LEU:HA	1.94	0.50
1:A:10:VAL:CG1	1:A:52:VAL:HG13	2.41	0.49
1:A:323:TYR:C	1:A:324:VAL:HG22	2.32	0.49
2:B:1695:THR:HA	2:B:1770:ASN:HB2	1.95	0.49
1:A:238:VAL:O	1:A:241:SER:N	2.44	0.49
1:A:663:VAL:HG13	2:B:1829:GLU:OE1	2.12	0.49
2:B:1739:THR:CB	2:B:1745:GLN:HB2	2.37	0.49
2:B:1940:ILE:HD11	2:B:1942:TRP:CE2	2.47	0.49
2:B:2262:ILE:HG13	2:B:2283:PHE:CE1	2.47	0.49
2:B:2284:GLN:OE1	2:B:2284:GLN:HA	2.12	0.49
2:B:1753:ASN:HA	2:B:1755:HIS:CE1	2.48	0.49
2:B:2265:SER:HB2	2:B:2271:TRP:CE3	2.47	0.49
1:A:186:LYS:O	1:A:190:GLN:CB	2.57	0.49
1:A:471:ARG:HD3	1:A:472:PRO:HD2	1.95	0.49
2:B:1706:LEU:HB3	2:B:1730:PHE:O	2.12	0.49
2:B:1957:HIS:HB3	2:B:1975:LEU:CB	2.43	0.49
1:A:197:LEU:HD13	1:A:255:TRP:HB3	1.93	0.49
1:A:234:VAL:C	1:A:236:GLY:N	2.66	0.49
1:A:645:GLN:C	1:A:647:ASP:H	2.16	0.49
2:B:1958:PHE:CD1	2:B:1998:VAL:HG12	2.47	0.49
2:B:2050:LEU:HB2	2:B:2055:TYR:CE2	2.47	0.49
1:A:156:TYR:HA	1:A:293:PHE:HE2	1.78	0.49
1:A:504:LEU:HB3	1:A:505:PRO:HD2	1.94	0.49
1:A:669:THR:HG21	2:B:1979:TYR:HB3	1.95	0.49
2:B:1871:VAL:N	2:B:1873:VAL:HG23	2.28	0.49
1:A:115:ASP:HA	1:A:123:LYS:HZ1	1.78	0.49
1:A:654:SER:HB3	1:A:688:TRP:HB3	1.95	0.49
1:A:690:LEU:HD12	1:A:704:ALA:HB3	1.94	0.49
2:B:1876:PHE:HD2	2:B:1940:ILE:HD13	1.78	0.49
1:A:666:ASP:OD2	1:A:666:ASP:C	2.51	0.49
1:A:520:GLY:HA2	1:A:529:LEU:HD11	1.95	0.48
1:A:534:SER:HB3	1:A:536:PHE:CE2	2.48	0.48
1:A:3:ARG:HH22	1:A:79:GLU:HG2	1.77	0.48
1:A:285:SER:O	1:A:285:SER:OG	2.27	0.48
1:A:127:LYS:HG2	1:A:162:VAL:HG22	1.94	0.48
1:A:293:PHE:N	1:A:293:PHE:HD1	2.12	0.48
1:A:604:GLU:HA	1:A:609:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:SER:HB3	2:B:1979:TYR:OH	2.14	0.48
2:B:1890:TYR:O	2:B:1893:GLU:HB2	2.13	0.48
2:B:1958:PHE:CD1	2:B:1998:VAL:CG1	2.96	0.48
2:B:2052:ARG:HD2	2:B:2052:ARG:N	2.29	0.48
1:A:284:ALA:HB2	1:A:531:ARG:NH2	2.29	0.48
1:A:604:GLU:HA	1:A:609:GLN:NE2	2.28	0.48
2:B:2104:MET:HG2	2:B:2114:THR:HA	1.95	0.48
1:A:64:PRO:C	1:A:66:PRO:HD2	2.34	0.48
1:A:202:PHE:H	1:A:202:PHE:HD1	1.57	0.48
1:A:113:GLU:O	1:A:114:TYR:HB3	2.14	0.48
1:A:194:LYS:HA	1:A:254:TYR:O	2.13	0.48
1:A:443:GLN:O	1:A:445:GLU:N	2.46	0.48
1:A:459:ASP:O	1:A:515:VAL:HG23	2.12	0.48
1:A:660:HIS:HB2	1:A:678:VAL:HG12	1.95	0.48
2:B:2075:LEU:HD22	2:B:2079:MET:HG3	1.96	0.48
1:A:8:GLY:HA2	1:A:88:LEU:HA	1.96	0.48
2:B:1935:ALA:O	2:B:1937:ASP:N	2.47	0.48
2:B:2260:PHE:O	2:B:2283:PHE:HB2	2.14	0.48
2:B:2107:LEU:HD12	2:B:2108:ASP:OD2	2.12	0.47
1:A:10:VAL:HG22	1:A:11:GLU:H	1.79	0.47
1:A:316:GLN:O	1:A:317:HIS:C	2.52	0.47
2:B:1732:LYS:HB3	2:B:1849:SER:O	2.14	0.47
2:B:2199:MET:HG3	2:B:2200:PHE:H	1.75	0.47
1:A:71:LEU:HD11	1:A:236:GLY:HA3	1.96	0.47
1:A:233:THR:HG21	1:A:319:GLY:O	2.15	0.47
2:B:1929:LEU:N	2:B:2012:THR:HG23	2.23	0.47
2:B:2149:ILE:HD12	2:B:2149:ILE:H	1.80	0.47
2:B:1781:ARG:HD2	2:B:1783:TYR:HE1	1.78	0.47
2:B:1837:TYR:CE1	2:B:1853:GLY:HA3	2.49	0.47
1:A:477:PRO:HG3	1:A:513:TRP:CD2	2.49	0.47
1:A:651:VAL:CG2	1:A:668:LEU:HB3	2.43	0.47
2:B:2087:GLN:OE1	2:B:2163:ARG:NE	2.45	0.47
1:A:186:LYS:HA	1:A:189:THR:HG22	1.96	0.47
1:A:279:ARG:C	1:A:281:HIS:N	2.67	0.47
2:B:1797:ARG:HA	2:B:1797:ARG:NH1	2.30	0.47
2:B:2087:GLN:HB3	2:B:2163:ARG:HG2	1.96	0.47
1:A:397:PRO:HD2	1:A:624:SER:OG	2.14	0.47
2:B:1785:PHE:HZ	2:B:1815:TYR:HB2	1.77	0.47
2:B:2237:THR:HB	2:B:2331:LEU:H	1.80	0.47
1:A:425:LYS:HE3	1:A:545:SER:C	2.35	0.47
2:B:2141:ASN:CB	2:B:2142:PRO:HD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2263:SER:OG	2:B:2307:ARG:HB2	2.15	0.47
1:A:453:LEU:CD2	1:A:513:TRP:HZ3	2.28	0.47
1:A:679:PHE:CD2	1:A:680:MET:N	2.83	0.47
2:B:1945:LEU:HD22	2:B:1983:PHE:HB3	1.97	0.47
1:A:238:VAL:HG12	1:A:239:ASN:N	2.29	0.46
2:B:2311:GLN:HA	2:B:2311:GLN:NE2	2.29	0.46
1:A:329:CYS:HA	1:A:330:PRO:HD3	1.86	0.46
1:A:424:LYS:HE2	1:A:593:ARG:HD3	1.96	0.46
2:B:1789:LEU:HB2	2:B:1823:MET:CE	2.45	0.46
2:B:1789:LEU:HD12	2:B:1823:MET:CG	2.45	0.46
2:B:2172:ASN:C	2:B:2174:CYS:H	2.18	0.46
2:B:2218:ALA:HB2	2:B:2248:VAL:HG12	1.97	0.46
1:A:198:LEU:CD2	1:A:200:ALA:HB2	2.45	0.46
1:A:272:GLU:N	1:A:272:GLU:CD	2.68	0.46
2:B:1742:SER:O	2:B:1743:PHE:C	2.53	0.46
2:B:2190:ILE:HG23	2:B:2231:GLN:O	2.15	0.46
1:A:102:GLY:HA2	2:B:1974:ALA:HB2	1.98	0.46
1:A:248:CYS:SG	1:A:330:PRO:HD2	2.55	0.46
1:A:393:TRP:HE3	1:A:394:ASP:N	2.13	0.46
2:B:2037:ILE:CG1	2:B:2040:SER:O	2.54	0.46
2:B:2276:GLN:HB3	2:B:2277:ASN:H	1.42	0.46
1:A:275:THR:HA	1:A:298:THR:HG22	1.96	0.46
1:A:393:TRP:CE3	1:A:394:ASP:N	2.84	0.46
1:A:690:LEU:HD22	1:A:691:GLY:N	2.31	0.46
2:B:1944:LEU:HD22	2:B:1956:ILE:HD13	1.97	0.46
2:B:1957:HIS:HB2	2:B:1974:ALA:O	2.15	0.46
2:B:1870:GLN:HA	2:B:1873:VAL:HB	1.97	0.46
1:A:512:LYS:HE3	1:A:514:THR:OG1	2.16	0.46
2:B:2047:ALA:CA	2:B:2062:TRP:CD1	2.82	0.46
2:B:2154:THR:O	2:B:2155:HIS:HB2	2.15	0.46
1:A:598:PRO:HB2	1:A:601:VAL:HG13	1.96	0.46
1:A:282:ARG:CZ	1:A:522:THR:HB	2.46	0.46
1:A:698:ARG:NH1	2:B:1843:LEU:HD11	2.31	0.46
2:B:1772:MET:HA	2:B:1816:PHE:HB2	1.98	0.46
2:B:1938:GLN:HG2	4:D:1:NAG:H61	1.98	0.46
2:B:2117:GLY:O	2:B:2118:ASN:C	2.55	0.46
2:B:2231:GLN:OE1	2:B:2271:TRP:CH2	2.69	0.46
2:B:2256:TYR:CE1	2:B:2287:GLN:HA	2.51	0.45
1:A:234:VAL:H	1:A:320:MET:HG2	1.82	0.45
2:B:2071:ILE:O	2:B:2150:ARG:HA	2.15	0.45
1:A:200:ALA:HA	1:A:260:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:HIS:O	1:A:300:LEU:HB2	2.16	0.45
1:A:411:TYR:C	1:A:421:ARG:HD3	2.36	0.45
1:A:624:SER:O	1:A:625:LEU:O	2.34	0.45
2:B:2064:THR:HG22	2:B:2066:GLU:HB2	1.98	0.45
2:B:2236:LYS:O	2:B:2304:ARG:HG3	2.16	0.45
1:A:157:SER:HB2	1:A:173:ILE:HD11	1.98	0.45
1:A:294:LEU:HD22	2:B:1973:MET:CE	2.47	0.45
1:A:395:TYR:HE2	1:A:614:MET:HG3	1.81	0.45
1:A:624:SER:O	1:A:625:LEU:C	2.54	0.45
1:A:409:SER:O	1:A:418:ARG:HG2	2.17	0.45
2:B:1883:PHE:HB2	2:B:1918:PHE:HB3	1.98	0.45
2:B:1884:ASP:HA	2:B:1914:GLU:CB	2.47	0.45
2:B:2205:PRO:C	2:B:2207:LYS:H	2.20	0.45
1:A:65:ARG:O	1:A:66:PRO:C	2.54	0.45
1:A:67:PRO:HB2	1:A:68:TRP:H	1.49	0.45
1:A:249:HIS:HB2	1:A:326:VAL:HG12	1.98	0.45
1:A:115:ASP:C	1:A:117:GLN:H	2.20	0.45
1:A:163:ASP:OD1	1:A:166:LYS:HB2	2.17	0.45
1:A:238:VAL:N	1:A:241:SER:HB2	2.31	0.45
2:B:1706:LEU:HG	2:B:1707:TRP:N	2.31	0.45
2:B:1707:TRP:CD1	2:B:1918:PHE:CE1	3.04	0.45
2:B:1823:MET:O	2:B:1857:VAL:HG11	2.17	0.45
1:A:411:TYR:O	1:A:421:ARG:NH1	2.45	0.45
1:A:467:ASN:ND2	1:A:472:PRO:HA	2.32	0.45
1:A:16:TYR:O	1:A:238:VAL:HG23	2.17	0.45
2:B:1833:LYS:HD3	2:B:1834:ALA:N	2.31	0.45
2:B:2311:GLN:HA	2:B:2311:GLN:HE21	1.82	0.45
1:A:80:VAL:HG13	1:A:180:ARG:HA	1.99	0.44
1:A:540:GLU:OE1	1:A:540:GLU:N	2.43	0.44
2:B:1820:GLN:HG3	2:B:1821:HIS:N	2.32	0.44
1:A:578:VAL:HB	1:A:644:ALA:HA	1.99	0.44
2:B:1783:TYR:O	2:B:1807:VAL:HB	2.17	0.44
1:A:90:ASN:O	1:A:131:GLY:HA2	2.17	0.44
1:A:94:HIS:CD2	1:A:95:PRO:HD2	2.52	0.44
1:A:402:PRO:HG2	1:A:419:ILE:HA	1.99	0.44
1:A:449:LEU:HD11	1:A:575:LEU:HB3	2.00	0.44
1:A:491:LEU:O	1:A:492:PRO:C	2.55	0.44
1:A:598:PRO:CB	1:A:601:VAL:HG13	2.47	0.44
1:A:697:PHE:C	1:A:699:ASN:H	2.20	0.44
2:B:1946:SER:HB2	2:B:1978:LEU:HD13	2.00	0.44
2:B:2087:GLN:HG2	2:B:2088:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:THR:HG21	1:A:286:LEU:CD2	2.46	0.44
1:A:435:THR:O	1:A:437:LYS:N	2.48	0.44
2:B:2041:GLY:HA2	2:B:2064:THR:OG1	2.18	0.44
2:B:2262:ILE:HG13	2:B:2283:PHE:HE1	1.83	0.44
2:B:1826:THR:H	2:B:1829:GLU:HB2	1.82	0.44
1:A:65:ARG:O	1:A:69:MET:HB2	2.18	0.44
1:A:570:LYS:HD2	1:A:571:ARG:HH21	1.82	0.44
2:B:1755:HIS:HB3	2:B:1931:GLY:O	2.18	0.44
2:B:2081:ILE:HG13	2:B:2144:ILE:HB	2.00	0.44
1:A:324:VAL:O	1:A:326:VAL:HG23	2.17	0.44
2:B:1893:GLU:O	2:B:1897:ARG:NH1	2.50	0.44
2:B:2120:THR:HG23	2:B:2121:GLY:N	2.28	0.44
2:B:2226:PRO:C	2:B:2228:GLU:H	2.21	0.44
1:A:393:TRP:CH2	1:A:620:TYR:CE1	3.06	0.44
1:A:412:LEU:HD22	1:A:421:ARG:HA	1.99	0.44
2:B:1956:ILE:H	2:B:1956:ILE:HG13	1.63	0.44
1:A:476:TYR:OH	1:A:483:VAL:HG13	2.18	0.43
2:B:1872:THR:HA	4:D:1:NAG:C6	2.47	0.43
2:B:1880:LEU:HD23	2:B:1880:LEU:N	2.33	0.43
2:B:1921:ILE:O	2:B:1922:ASN:CB	2.56	0.43
2:B:1940:ILE:HD11	2:B:1942:TRP:CD2	2.52	0.43
2:B:1969:GLU:HB3	2:B:1970:GLU:H	1.54	0.43
1:A:67:PRO:HG2	1:A:68:TRP:CD1	2.53	0.43
1:A:97:SER:OG	1:A:161:HIS:N	2.51	0.43
1:A:137:VAL:O	1:A:137:VAL:HG23	2.18	0.43
2:B:1922:ASN:HB3	2:B:1925:ILE:HD11	1.99	0.43
2:B:1964:THR:HB	2:B:1972:LYS:HD2	2.00	0.43
1:A:412:LEU:HD12	1:A:423:TYR:CE1	2.53	0.43
2:B:1957:HIS:HB3	2:B:1975:LEU:HB3	2.00	0.43
2:B:1961:HIS:ND1	2:B:2014:PHE:HZ	2.17	0.43
1:A:305:GLN:HB2	1:A:323:TYR:HB3	2.00	0.43
1:A:309:PHE:HB3	1:A:311:HIS:HB2	2.00	0.43
1:A:509:PHE:HD1	1:A:510:LYS:N	2.16	0.43
2:B:2096:LEU:HA	2:B:2157:SER:CB	2.49	0.43
1:A:605:ASP:O	1:A:609:GLN:HG2	2.19	0.43
2:B:1706:LEU:HD22	2:B:1732:LYS:N	2.14	0.43
2:B:1897:ARG:NH1	2:B:1897:ARG:HB3	2.33	0.43
1:A:159:LEU:CD1	1:A:160:SER:H	2.28	0.43
2:B:1737:GLU:OE2	2:B:1761:PRO:HB2	2.19	0.43
2:B:2255:MET:HB3	2:B:2318:ALA:CB	2.48	0.43
1:A:50:LEU:HD23	1:A:51:PHE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LYS:H	1:A:380:LYS:HG2	1.73	0.43
1:A:471:ARG:HG3	1:A:585:TRP:CZ3	2.54	0.43
2:B:1756:LEU:C	2:B:1922:ASN:HD21	2.22	0.43
2:B:1869:ARG:O	2:B:1870:GLN:HB3	2.18	0.43
2:B:1870:GLN:O	2:B:1872:THR:N	2.52	0.43
2:B:1706:LEU:HD13	2:B:1732:LYS:CB	2.43	0.42
2:B:1807:VAL:HG22	2:B:1813:LYS:HB2	2.01	0.42
2:B:2291:THR:HA	2:B:2292:PRO:HD3	1.84	0.42
1:A:289:SER:O	1:A:290:PRO:C	2.57	0.42
1:A:640:LEU:HD12	1:A:640:LEU:N	2.33	0.42
1:A:711:CYS:HB3	1:A:712:ASP:H	1.52	0.42
2:B:1703:VAL:HG12	2:B:1704:GLU:H	1.83	0.42
2:B:2210:LEU:CD1	2:B:2244:THR:HG22	2.46	0.42
1:A:453:LEU:HD23	1:A:513:TRP:HZ3	1.84	0.42
1:A:585:TRP:C	1:A:586:TYR:CD1	2.93	0.42
2:B:1853:GLY:HA2	2:B:1854:PRO:HD3	1.87	0.42
2:B:1921:ILE:HD11	2:B:2010:MET:HG3	2.00	0.42
2:B:1953:ILE:H	2:B:1953:ILE:HG13	1.72	0.42
2:B:2001:LEU:HD12	2:B:2001:LEU:HA	1.81	0.42
2:B:2084:ILE:O	2:B:2084:ILE:HG23	2.20	0.42
2:B:2218:ALA:CB	2:B:2248:VAL:HG12	2.45	0.42
2:B:2309:HIS:HA	2:B:2310:PRO:HD2	1.89	0.42
1:A:269:ILE:C	1:A:270:PHE:CD2	2.93	0.42
1:A:282:ARG:CD	1:A:522:THR:HG21	2.49	0.42
1:A:632:HIS:N	1:A:682:MET:O	2.53	0.42
1:A:652:PHE:HB3	1:A:691:GLY:H	1.84	0.42
2:B:1790:ILE:HG12	2:B:1792:TYR:CE2	2.53	0.42
2:B:1957:HIS:HB3	2:B:1975:LEU:HB2	2.01	0.42
1:A:155:THR:HB	1:A:293:PHE:HB2	2.02	0.42
1:A:165:VAL:HG13	1:A:262:THR:OG1	2.19	0.42
1:A:300:LEU:HB3	1:A:326:VAL:CG1	2.50	0.42
1:A:495:VAL:HG11	1:A:501:PHE:HB2	2.01	0.42
1:A:3:ARG:O	1:A:84:VAL:HA	2.19	0.42
1:A:80:VAL:HG23	1:A:181:GLU:HG3	2.02	0.42
1:A:87:THR:CG2	1:A:135:THR:HG23	2.42	0.42
1:A:115:ASP:HA	1:A:123:LYS:NZ	2.34	0.42
1:A:666:ASP:OD1	2:B:1788:SER:OG	2.36	0.42
1:A:684:ASN:HA	1:A:685:PRO:HD2	1.90	0.42
2:B:1834:ALA:CB	2:B:1943:TYR:HD2	2.27	0.42
2:B:2145:ILE:H	2:B:2145:ILE:HG13	1.72	0.42
1:A:65:ARG:N	1:A:66:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:HB2	2:B:1995:ILE:O	2.19	0.42
1:A:246:ILE:HG12	1:A:325:LYS:C	2.40	0.42
1:A:521:PRO:C	1:A:522:THR:CG2	2.87	0.42
2:B:2032:ILE:O	2:B:2033:ARG:HG3	2.20	0.42
2:B:2081:ILE:O	2:B:2140:PHE:HD2	2.03	0.42
2:B:2090:ARG:HB2	2:B:2132:SER:HB3	2.01	0.42
2:B:2256:TYR:CE1	2:B:2314:VAL:HB	2.55	0.42
1:A:85:VAL:O	1:A:85:VAL:CG1	2.67	0.42
1:A:412:LEU:HB2	1:A:421:ARG:CB	2.50	0.42
1:A:417:GLN:HB2	1:A:596:PRO:HD3	2.02	0.42
1:A:480:ILE:HG22	1:A:481:THR:N	2.35	0.42
2:B:1699:PHE:CD1	2:B:1699:PHE:N	2.88	0.42
2:B:1707:TRP:CD1	2:B:1918:PHE:HE1	2.38	0.42
2:B:1707:TRP:HZ3	2:B:1709:TYR:HB2	1.83	0.42
2:B:1880:LEU:HD22	2:B:1921:ILE:HG12	2.02	0.42
2:B:2033:ARG:NE	2:B:2049:LYS:HG2	2.35	0.42
1:A:198:LEU:HD22	1:A:200:ALA:HB2	2.01	0.42
2:B:1913:LYS:HE2	2:B:1913:LYS:HB3	1.81	0.42
2:B:2250:SER:C	2:B:2252:LEU:N	2.73	0.42
2:B:2331:LEU:HB3	2:B:2332:TYR:CE2	2.55	0.42
1:A:291:ILE:O	2:B:1977:ASN:ND2	2.53	0.41
2:B:1698:TYR:CD1	2:B:1763:ILE:HG23	2.55	0.41
2:B:1929:LEU:CD2	2:B:2012:THR:CG2	2.97	0.41
2:B:2037:ILE:CG1	2:B:2038:THR:N	2.67	0.41
2:B:2237:THR:O	2:B:2327:GLU:HB2	2.20	0.41
1:A:393:TRP:CE3	1:A:393:TRP:CA	2.98	0.41
1:A:492:PRO:C	1:A:494:GLY:H	2.17	0.41
1:A:663:VAL:CG1	1:A:664:TYR:N	2.84	0.41
2:B:1925:ILE:HD13	2:B:1925:ILE:N	2.35	0.41
2:B:1946:SER:H	2:B:1978:LEU:HD22	1.85	0.41
2:B:2042:GLN:O	2:B:2043:TYR:HB2	2.20	0.41
2:B:2048:PRO:HD3	2:B:2062:TRP:CG	2.55	0.41
2:B:2061:ALA:HB1	2:B:2162:LEU:O	2.20	0.41
1:A:260:MET:HG3	1:A:261:GLY:N	2.35	0.41
1:A:276:PHE:CZ	1:A:518:GLU:O	2.72	0.41
1:A:524:SER:O	2:B:1968:LYS:HE3	2.20	0.41
2:B:1709:TYR:O	2:B:1710:GLY:C	2.59	0.41
2:B:1739:THR:HG21	2:B:1745:GLN:HG3	2.01	0.41
1:A:52:VAL:HB	1:A:53:GLU:H	1.71	0.41
1:A:65:ARG:H	1:A:65:ARG:HG3	1.40	0.41
1:A:305:GLN:HA	1:A:324:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:PHE:CE2	1:A:475:ILE:HG23	2.55	0.41
1:A:626:GLN:HB2	1:A:705:LEU:C	2.40	0.41
2:B:1900:ARG:HB2	2:B:1902:PRO:HD2	2.03	0.41
2:B:2293:VAL:O	2:B:2295:ASN:N	2.53	0.41
1:A:168:LEU:O	1:A:171:GLY:N	2.54	0.41
1:A:446:SER:O	1:A:449:LEU:HB2	2.21	0.41
1:A:460:THR:HG23	1:A:514:THR:HG23	2.02	0.41
2:B:1897:ARG:HG2	2:B:1898:ASN:N	2.36	0.41
2:B:1912:PHE:O	2:B:1916:TYR:N	2.53	0.41
2:B:2043:TYR:HB2	2:B:2063:SER:O	2.20	0.41
1:A:56:ASP:HB2	1:A:58:LEU:O	2.20	0.41
1:A:615:HIS:O	1:A:621:VAL:HG23	2.20	0.41
2:B:1921:ILE:O	2:B:1921:ILE:CG2	2.64	0.41
2:B:2048:PRO:HD3	2:B:2062:TRP:HB2	2.02	0.41
1:A:232:HIS:HE1	1:A:267:HIS:HE1	1.66	0.41
1:A:270:PHE:CD2	1:A:270:PHE:N	2.88	0.41
2:B:1774:THR:HG23	2:B:1814:THR:HB	2.03	0.41
1:A:127:LYS:HE2	1:A:162:VAL:HG13	2.03	0.41
1:A:303:LEU:O	1:A:304:GLY:C	2.58	0.41
2:B:1747:LEU:O	2:B:1748:TYR:C	2.59	0.41
2:B:1876:PHE:CD2	2:B:1940:ILE:HD13	2.56	0.41
2:B:1929:LEU:HD23	2:B:2012:THR:HG22	2.02	0.41
1:A:141:LEU:H	1:A:144:ASN:ND2	2.18	0.41
1:A:156:TYR:O	1:A:176:LEU:O	2.39	0.41
1:A:382:TRP:HB2	1:A:461:LEU:HD12	2.01	0.41
1:A:476:TYR:CZ	1:A:483:VAL:HG11	2.55	0.41
1:A:532:TYR:HA	1:A:551:LEU:H	1.86	0.41
2:B:1778:GLN:HE21	2:B:1778:GLN:HB2	1.71	0.41
2:B:2027:MET:O	2:B:2052:ARG:HG2	2.20	0.41
2:B:2100:GLN:HB3	2:B:2154:THR:HB	2.02	0.41
2:B:2176:MET:HA	2:B:2177:PRO:HD2	1.80	0.41
1:A:307:LEU:H	1:A:307:LEU:HG	1.63	0.41
1:A:538:ASN:OD1	1:A:541:ARG:HB3	2.21	0.41
1:A:578:VAL:HG23	1:A:644:ALA:HB2	2.02	0.41
2:B:2209:ARG:HB2	2:B:2212:LEU:HD13	2.02	0.41
1:A:113:GLU:HG2	1:A:126:ASP:HB3	2.04	0.40
1:A:449:LEU:HD22	1:A:550:PRO:HD3	2.02	0.40
1:A:498:LEU:C	1:A:500:ASP:N	2.74	0.40
1:A:524:SER:O	1:A:525:ASP:O	2.39	0.40
2:B:1829:GLU:HB3	2:B:1830:PHE:H	1.65	0.40
2:B:1884:ASP:HA	2:B:1914:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PHE:CD2	1:A:269:ILE:HG12	2.50	0.40
1:A:233:THR:HG22	1:A:320:MET:CG	2.52	0.40
1:A:290:PRO:HB2	1:A:291:ILE:H	1.76	0.40
1:A:426:VAL:HG11	1:A:473:TYR:OH	2.22	0.40
1:A:477:PRO:HD3	1:A:513:TRP:CZ2	2.56	0.40
1:A:688:TRP:HB2	1:A:706:LEU:HG	2.02	0.40
2:B:1926:MET:HB2	2:B:1927:ASP:H	1.56	0.40
2:B:1945:LEU:HD13	2:B:1983:PHE:HB3	2.02	0.40
2:B:2040:SER:O	2:B:2040:SER:OG	2.38	0.40
2:B:1789:LEU:H	2:B:1823:MET:HE2	1.86	0.40
2:B:2087:GLN:HG2	2:B:2088:GLY:N	2.35	0.40
1:A:303:LEU:O	1:A:303:LEU:HD23	2.22	0.40
1:A:471:ARG:HD2	1:A:585:TRP:CH2	2.56	0.40
2:B:1777:ASN:ND2	2:B:1782:PRO:HA	2.35	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	622/754 (82%)	430 (69%)	130 (21%)	62 (10%)	0 9
2	B	627/684 (92%)	437 (70%)	126 (20%)	64 (10%)	0 9
All	All	1249/1438 (87%)	867 (69%)	256 (20%)	126 (10%)	0 9

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	THR
1	A	133	SER
1	A	181	GLU
1	A	227	ALA

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Mol	Chain	Res	Type
1	A	232	HIS
1	A	243	PRO
1	A	290	PRO
1	A	316	GLN
1	A	326	VAL
1	A	378	HIS
1	A	419	ILE
1	A	444	HIS
1	A	492	PRO
1	A	493	LYS
1	A	525	ASP
1	A	604	GLU
1	A	671	PHE
2	B	1706	LEU
2	B	1791	SER
2	B	1889	TRP
2	B	1910	PRO
2	B	1926	MET
2	B	1930	PRO
2	B	1967	LYS
2	B	2003	GLY
2	B	2044	GLY
2	B	2047	ALA
2	B	2061	ALA
2	B	2110	LYS
2	B	2291	THR
2	B	2294	VAL
1	A	46	TYR
1	A	67	PRO
1	A	80	VAL
1	A	114	TYR
1	A	182	GLY
1	A	184	LEU
1	A	235	ASN
1	A	239	ASN
1	A	303	LEU
1	A	304	GLY
1	A	324	VAL
1	A	501	PHE
1	A	561	GLN
1	A	570	LYS
1	A	587	LEU

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Mol	Chain	Res	Type
1	A	593	ARG
1	A	596	PRO
1	A	601	VAL
1	A	625	LEU
1	A	626	GLN
2	B	1705	ARG
2	B	1710	GLY
2	B	1743	PHE
2	B	1757	GLY
2	B	1843	LEU
2	B	1870	GLN
2	B	1871	VAL
2	B	1888	SER
2	B	1912	PHE
2	B	1922	ASN
2	B	1936	GLN
2	B	1938	GLN
2	B	1977	ASN
2	B	1991	SER
2	B	2034	ASP
2	B	2037	ILE
2	B	2039	ALA
2	B	2043	TYR
2	B	2049	LYS
2	B	2117	GLY
2	B	2119	SER
2	B	2120	THR
2	B	2137	HIS
2	B	2208	ALA
2	B	2210	LEU
2	B	2251	LEU
2	B	2252	LEU
1	A	62	ALA
1	A	68	TRP
1	A	148	ALA
1	A	151	PRO
1	A	225	ALA
1	A	397	PRO
1	A	403	ASP
1	A	416	PRO
1	A	498	LEU
1	A	585	TRP

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Mol	Chain	Res	Type
2	B	1748	TYR
2	B	1767	VAL
2	B	1867	HIS
2	B	1928	THR
2	B	2276	GLN
1	A	61	ILE
1	A	204	GLU
1	A	264	PRO
1	A	275	THR
1	A	435	THR
1	A	672	PRO
1	A	674	SER
2	B	1780	SER
2	B	1846	ASP
2	B	2011	SER
2	B	2114	THR
2	B	2329	GLN
1	A	412	LEU
1	A	503	ILE
1	A	521	PRO
1	A	653	PHE
2	B	1712	SER
2	B	1789	LEU
2	B	1802	PRO
2	B	1906	GLN
2	B	2038	THR
2	B	2045	GLN
2	B	2326	CYS
1	A	413	ASN
1	A	698	ARG
2	B	2160	SER
2	B	2128	GLY
2	B	2135	ILE
1	A	494	GLY
2	B	1873	VAL
2	B	2059	ILE
1	A	171	GLY
2	B	1850	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	559/674 (83%)	414 (74%)	145 (26%)	0 4
2	B	560/612 (92%)	446 (80%)	114 (20%)	1 7
All	All	1119/1286 (87%)	860 (77%)	259 (23%)	1 5

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	10	VAL
1	A	13	SER
1	A	16	TYR
1	A	45	VAL
1	A	50	LEU
1	A	51	PHE
1	A	52	VAL
1	A	54	PHE
1	A	56	ASP
1	A	57	HIS
1	A	59	PHE
1	A	65	ARG
1	A	71	LEU
1	A	80	VAL
1	A	82	ASP
1	A	83	THR
1	A	91	MET
1	A	94	HIS
1	A	101	VAL
1	A	105	TYR
1	A	107	LYS
1	A	113	GLU
1	A	118	THR
1	A	120	GLN
1	A	129	PHE
1	A	133	SER

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Mol	Chain	Res	Type
1	A	140	VAL
1	A	141	LEU
1	A	144	ASN
1	A	154	LEU
1	A	155	THR
1	A	161	HIS
1	A	168	LEU
1	A	170	SER
1	A	176	LEU
1	A	179	CYS
1	A	184	LEU
1	A	186	LYS
1	A	191	THR
1	A	196	ILE
1	A	202	PHE
1	A	204	GLU
1	A	206	LYS
1	A	209	HIS
1	A	224	SER
1	A	226	ARG
1	A	233	THR
1	A	234	VAL
1	A	241	SER
1	A	242	LEU
1	A	248	CYS
1	A	251	LYS
1	A	252	SER
1	A	255	TRP
1	A	257	VAL
1	A	260	MET
1	A	270	PHE
1	A	275	THR
1	A	276	PHE
1	A	277	LEU
1	A	282	ARG
1	A	286	LEU
1	A	292	THR
1	A	293	PHE
1	A	295	THR
1	A	302	ASP
1	A	307	LEU
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	312	ILE
1	A	316	GLN
1	A	324	VAL
1	A	328	SER
1	A	380	LYS
1	A	383	VAL
1	A	392	ASP
1	A	393	TRP
1	A	405	ARG
1	A	407	TYR
1	A	412	LEU
1	A	421	ARG
1	A	425	LYS
1	A	427	ARG
1	A	429	MET
1	A	432	THR
1	A	435	THR
1	A	437	LYS
1	A	438	THR
1	A	442	ILE
1	A	444	HIS
1	A	460	THR
1	A	463	ILE
1	A	475	ILE
1	A	483	VAL
1	A	484	ARG
1	A	486	LEU
1	A	490	ARG
1	A	497	HIS
1	A	500	ASP
1	A	509	PHE
1	A	515	VAL
1	A	517	VAL
1	A	519	ASP
1	A	524	SER
1	A	529	LEU
1	A	539	MET
1	A	542	ASP
1	A	543	LEU
1	A	545	SER
1	A	551	LEU
1	A	552	LEU

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Mol	Chain	Res	Type
1	A	558	SER
1	A	567	MET
1	A	571	ARG
1	A	573	VAL
1	A	583	ARG
1	A	584	SER
1	A	585	TRP
1	A	588	THR
1	A	593	ARG
1	A	597	ASN
1	A	601	VAL
1	A	602	GLN
1	A	604	GLU
1	A	617	ILE
1	A	623	ASP
1	A	626	GLN
1	A	627	LEU
1	A	629	VAL
1	A	631	LEU
1	A	639	ILE
1	A	640	LEU
1	A	642	ILE
1	A	645	GLN
1	A	650	SER
1	A	652	PHE
1	A	666	ASP
1	A	668	LEU
1	A	674	SER
1	A	683	GLU
1	A	690	LEU
1	A	696	ASP
1	A	698	ARG
1	A	708	VAL
1	A	712	ASP
2	B	1695	THR
2	B	1697	HIS
2	B	1703	VAL
2	B	1704	GLU
2	B	1727	VAL
2	B	1729	GLN
2	B	1733	VAL
2	B	1744	THR

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Mol	Chain	Res	Type
2	B	1747	LEU
2	B	1752	LEU
2	B	1758	LEU
2	B	1759	LEU
2	B	1769	ASP
2	B	1787	SER
2	B	1793	GLU
2	B	1797	ARG
2	B	1798	GLN
2	B	1814	THR
2	B	1815	TYR
2	B	1816	PHE
2	B	1822	HIS
2	B	1823	MET
2	B	1827	LYS
2	B	1832	CYS
2	B	1843	LEU
2	B	1847	VAL
2	B	1860	THR
2	B	1861	ASN
2	B	1869	ARG
2	B	1879	PHE
2	B	1880	LEU
2	B	1887	LYS
2	B	1889	TRP
2	B	1897	ARG
2	B	1898	ASN
2	B	1900	ARG
2	B	1907	MET
2	B	1908	GLU
2	B	1912	PHE
2	B	1916	TYR
2	B	1926	MET
2	B	1929	LEU
2	B	1934	MET
2	B	1938	GLN
2	B	1939	ARG
2	B	1940	ILE
2	B	1945	LEU
2	B	1951	GLU
2	B	1956	ILE
2	B	1957	HIS

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Mol	Chain	Res	Type
2	B	1963	PHE
2	B	1965	VAL
2	B	1966	ARG
2	B	1967	LYS
2	B	1971	TYR
2	B	1975	LEU
2	B	1977	ASN
2	B	1991	SER
2	B	1995	ILE
2	B	1997	ARG
2	B	1998	VAL
2	B	2006	LEU
2	B	2010	MET
2	B	2013	LEU
2	B	2014	PHE
2	B	2015	LEU
2	B	2031	HIS
2	B	2037	ILE
2	B	2046	TRP
2	B	2050	LEU
2	B	2052	ARG
2	B	2058	SER
2	B	2064	THR
2	B	2073	VAL
2	B	2085	LYS
2	B	2086	THR
2	B	2090	ARG
2	B	2091	GLN
2	B	2092	LYS
2	B	2098	ILE
2	B	2106	SER
2	B	2107	LEU
2	B	2111	LYS
2	B	2113	GLN
2	B	2122	THR
2	B	2130	VAL
2	B	2132	SER
2	B	2135	ILE
2	B	2136	LYS
2	B	2141	ASN
2	B	2149	ILE
2	B	2154	THR

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Mol	Chain	Res	Type
2	B	2156	TYR
2	B	2163	ARG
2	B	2164	MET
2	B	2166	LEU
2	B	2172	ASN
2	B	2175	SER
2	B	2178	LEU
2	B	2206	SER
2	B	2223	VAL
2	B	2249	LYS
2	B	2262	ILE
2	B	2270	GLN
2	B	2273	LEU
2	B	2277	ASN
2	B	2294	VAL
2	B	2301	LEU
2	B	2312	SER
2	B	2322	GLU
2	B	2327	GLU
2	B	2329	GLN
2	B	2330	ASP
2	B	2332	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	90	ASN
1	A	144	ASN
1	A	169	ASN
1	A	281	HIS
1	A	297	GLN
1	A	413	ASN
1	A	592	GLN
1	A	609	GLN
1	A	694	ASN
2	B	1736	GLN
2	B	1770	ASN
2	B	1778	GLN
2	B	1805	ASN
2	B	1820	GLN
2	B	1822	HIS

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Mol	Chain	Res	Type
2	B	1861	ASN
2	B	1864	ASN
2	B	1867	HIS
2	B	1898	ASN
2	B	1922	ASN
2	B	2036	GLN
2	B	2042	GLN
2	B	2129	ASN
2	B	2266	GLN
2	B	2311	GLN
2	B	2329	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	3,1	14,14,15	0.87	0	17,19,21	1.08	1 (5%)
3	NAG	C	2	3	14,14,15	2.88	3 (21%)	17,19,21	1.74	2 (11%)
4	NAG	D	1	4	14,14,15	0.95	0	17,19,21	1.63	6 (35%)
4	MAN	D	2	4	11,11,12	0.65	0	15,15,17	1.64	2 (13%)
4	MAN	D	3	4	11,11,12	0.70	0	15,15,17	1.99	2 (13%)
4	MAN	D	4	4	11,11,12	0.80	0	15,15,17	1.70	3 (20%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O7-C7	8.00	1.41	1.23
3	C	2	NAG	C8-C7	-6.01	1.38	1.50
3	C	2	NAG	C1-C2	2.69	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3	MAN	C1-O5-C5	6.47	120.96	112.19
3	C	2	NAG	C4-C3-C2	5.16	118.58	111.02
4	D	2	MAN	C1-O5-C5	4.51	118.30	112.19
4	D	4	MAN	C1-C2-C3	3.86	114.42	109.67
4	D	4	MAN	C2-C3-C4	3.79	117.45	110.89
4	D	4	MAN	C3-C4-C5	3.11	115.80	110.24
3	C	1	NAG	C4-C3-C2	3.00	115.42	111.02
4	D	1	NAG	C4-C3-C2	2.85	115.19	111.02
4	D	1	NAG	O4-C4-C3	2.73	116.67	110.35
3	C	2	NAG	C2-N2-C7	2.59	126.60	122.90
4	D	2	MAN	C3-C4-C5	2.50	114.70	110.24
4	D	3	MAN	C3-C4-C5	2.50	114.70	110.24
4	D	1	NAG	O5-C5-C6	2.45	111.05	107.20
4	D	1	NAG	C2-N2-C7	2.45	126.39	122.90
4	D	1	NAG	C1-O5-C5	-2.24	109.15	112.19
4	D	1	NAG	O7-C7-C8	-2.11	118.14	122.06

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	2	MAN	C1
4	D	4	MAN	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C3-C2-N2-C7
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	3	MAN	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
4	D	2	MAN	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	D	2	MAN	O5-C5-C6-O6

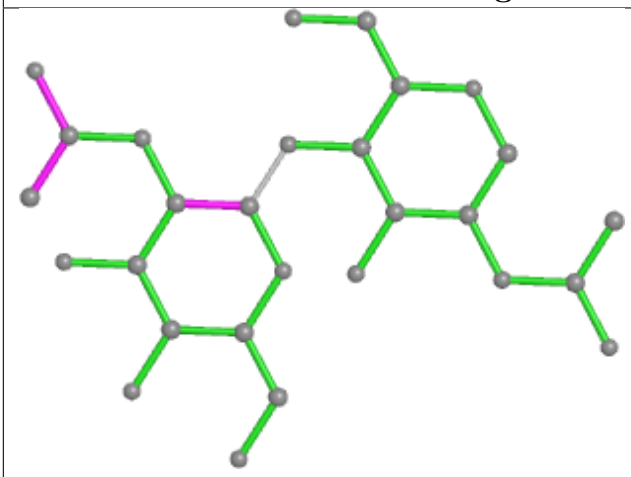
There are no ring outliers.

2 monomers are involved in 3 short contacts:

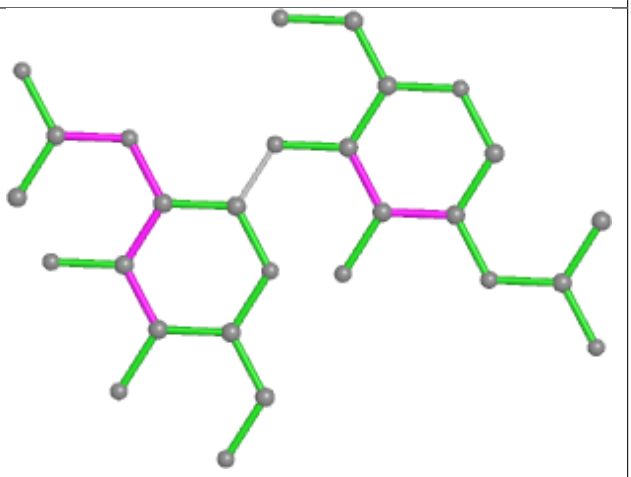
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
4	D	1	NAG	2	0

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

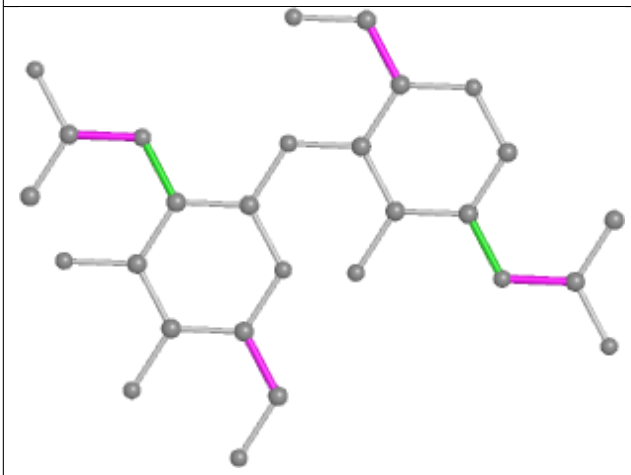
Oligosaccharide Chain C



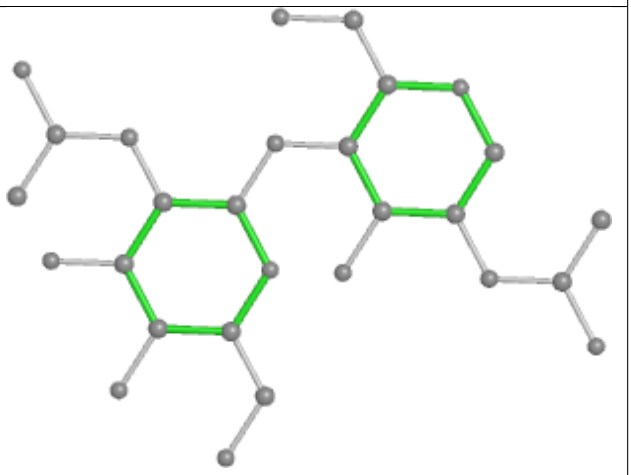
Bond lengths



Bond angles

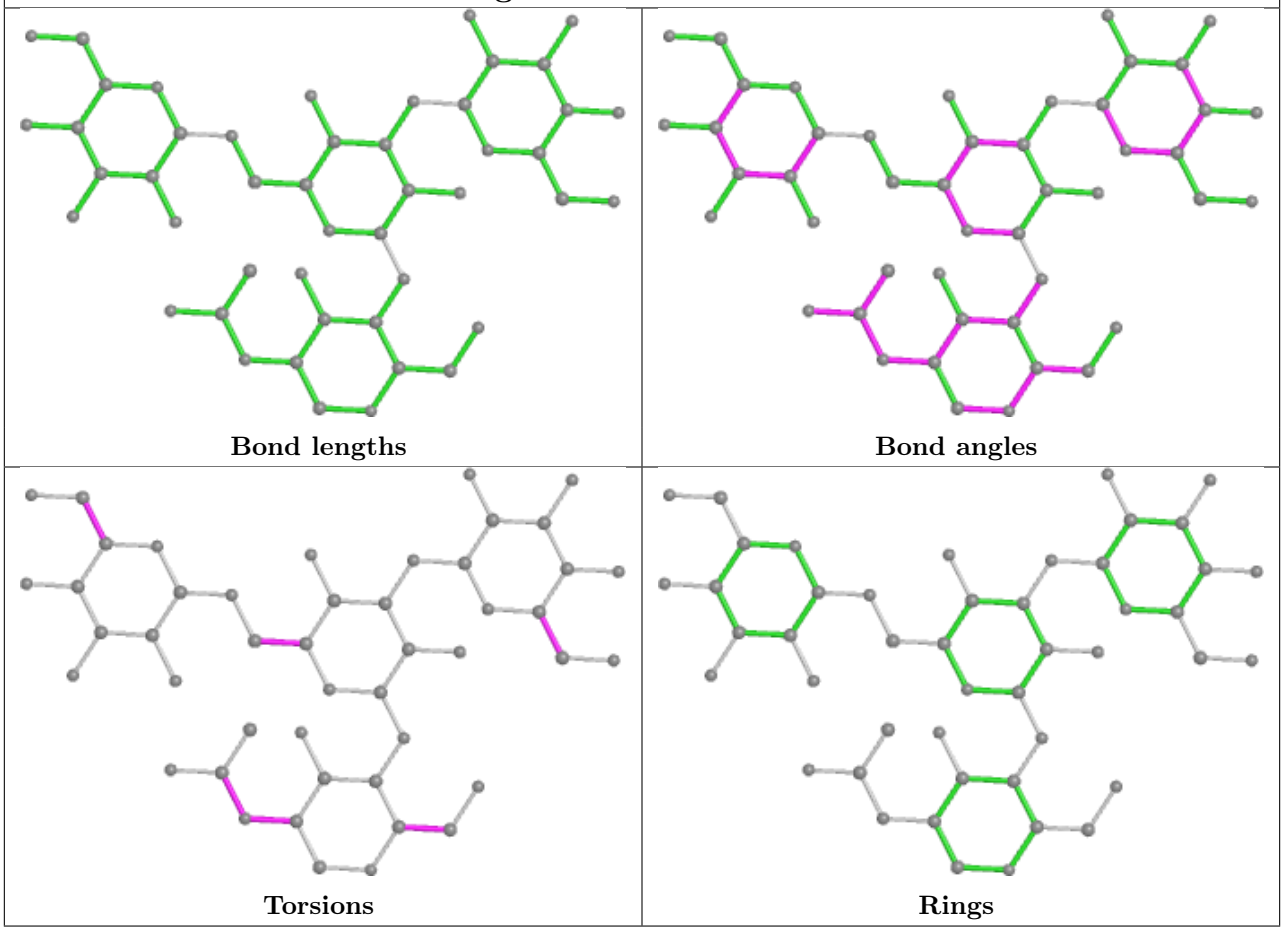


Torsions



Rings

Oligosaccharide Chain D



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	NAG	B	2334	2	14,14,15	0.84	0	17,19,21	1.25	2 (11%)
7	NAG	B	2333	2	14,14,15	0.76	0	17,19,21	2.03	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	2334	2	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	B	2333	2	1/1/5/7	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	2333	NAG	C1-O5-C5	5.06	119.05	112.19
7	B	2333	NAG	C3-C4-C5	4.43	118.14	110.24
7	B	2334	NAG	C1-O5-C5	2.99	116.25	112.19
7	B	2333	NAG	C2-N2-C7	2.54	126.52	122.90
7	B	2334	NAG	C2-N2-C7	2.47	126.42	122.90
7	B	2333	NAG	O5-C5-C4	2.45	116.78	110.83
7	B	2333	NAG	C4-C3-C2	2.17	114.20	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	2333	NAG	C1
7	B	2334	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2333	NAG	C8-C7-N2-C2
7	B	2333	NAG	O7-C7-N2-C2
7	B	2334	NAG	C8-C7-N2-C2
7	B	2334	NAG	O7-C7-N2-C2
7	B	2334	NAG	O5-C5-C6-O6
7	B	2334	NAG	C4-C5-C6-O6
7	B	2333	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	630/754 (83%)	0.14	18 (2%)	51	41	182, 196, 215, 239	0
2	B	631/684 (92%)	0.11	18 (2%)	51	41	181, 198, 214, 231	1 (0%)
All	All	1261/1438 (87%)	0.13	36 (2%)	51	41	181, 197, 215, 239	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1901	ALA	4.2
2	B	1902	PRO	4.0
1	A	333	PRO	3.9
2	B	2038	THR	3.3
2	B	2093	PHE	2.9
1	A	6	TYR	2.8
1	A	594	PHE	2.8
1	A	50	LEU	2.7
1	A	224	SER	2.7
1	A	11	GLU	2.6
2	B	1977	ASN	2.6
1	A	675	GLY	2.6
2	B	1693	LYS	2.6
1	A	395	TYR	2.5
1	A	71	LEU	2.5
1	A	569	ASP	2.5
1	A	12	LEU	2.5
2	B	2089	ALA	2.4
2	B	2243	VAL	2.3
1	A	88	LEU	2.3
1	A	49	THR	2.3
1	A	202	PHE	2.3
2	B	2295	ASN	2.3
1	A	10	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	2103	ILE	2.3
1	A	48	LYS	2.3
2	B	1800	ALA	2.3
2	B	1946	SER	2.3
2	B	2318	ALA	2.2
1	A	568	SER	2.1
2	B	1917	ARG	2.1
2	B	1950	ASN	2.1
2	B	2306	LEU	2.1
2	B	1900	ARG	2.0
2	B	1949	SER	2.0
1	A	45	VAL	2.0

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

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

6.3 Carbohydrates (i)

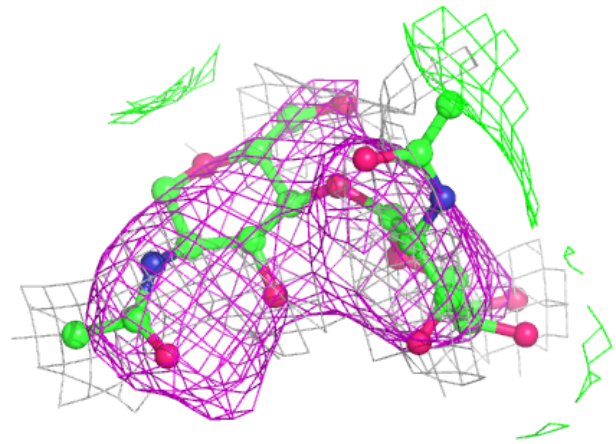
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

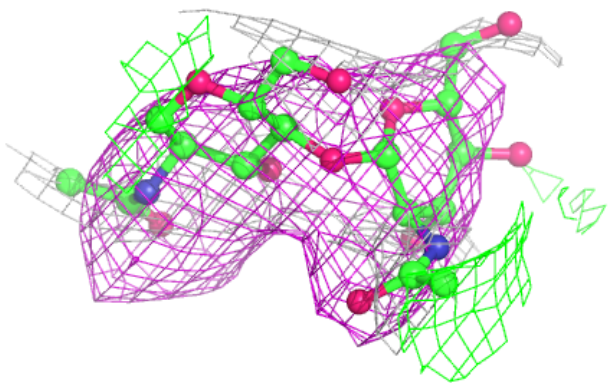
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	D	2	11/12	0.40	0.26	257,259,260,261	0
4	MAN	D	3	11/12	0.56	0.28	258,261,261,261	0
3	NAG	C	2	14/15	0.58	0.40	227,229,230,231	0
4	MAN	D	4	11/12	0.68	0.27	254,255,256,256	0
3	NAG	C	1	14/15	0.72	0.34	210,216,218,222	0
4	NAG	D	1	14/15	0.77	0.30	257,257,257,258	0

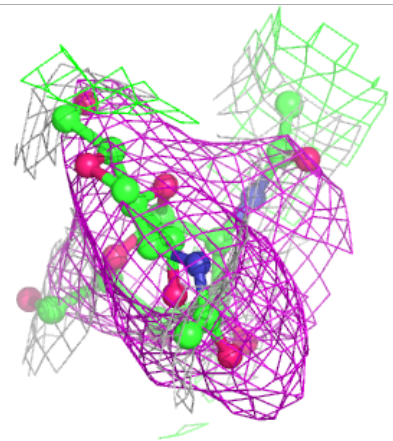
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

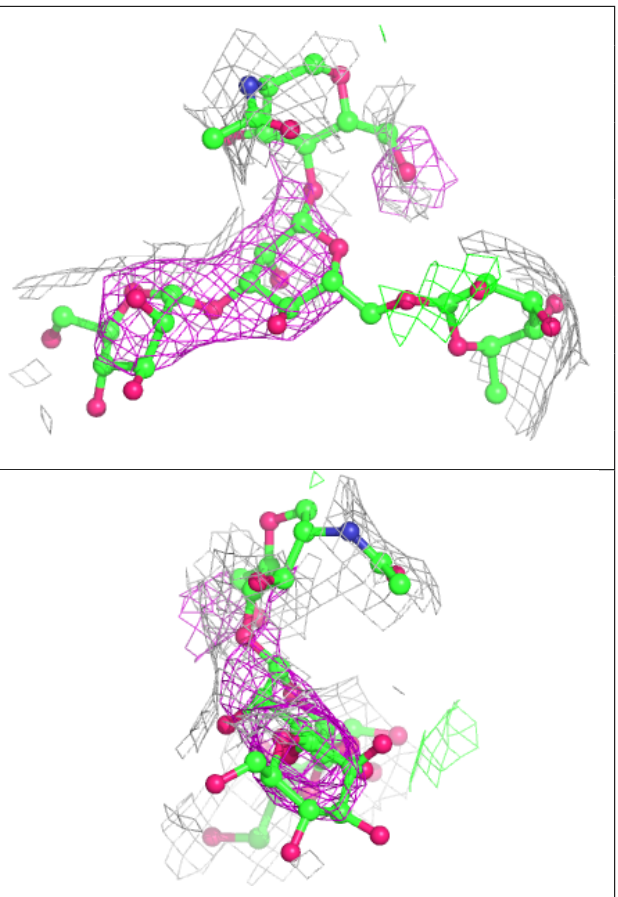






Electron density around Chain D:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	B	2333	14/15	0.86	0.49	210,213,214,214	0
7	NAG	B	2334	14/15	0.90	0.20	191,194,196,197	0
6	CA	A	758	1/1	0.91	0.13	172,172,172,172	0
5	CU	B	1	1/1	0.95	0.18	174,174,174,174	0
5	CU	A	757	1/1	1.00	0.16	171,171,171,171	0

6.5 Other polymers (i)

There are no such residues in this entry.