



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:28 PM UTC

PDB ID : 6TS2 / pdb_00006ts2
Title : Truncated version of Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) lacking domain TRXL2 (417-650).
Authors : Roversi, P.; Zitzmann, N.
Deposited on : 2019-12-19
Resolution : 5.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

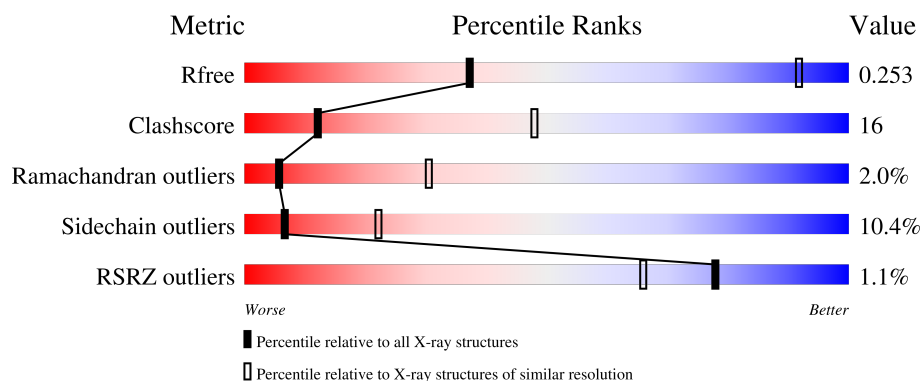
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (7.46-4.00)
Clashscore	190562	1171 (7.46-4.00)
Ramachandran outliers	187476	1005 (7.40-4.00)
Sidechain outliers	187428	1004 (7.50-3.98)
RSRZ outliers	180081	1103 (7.46-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	1260	2% 59% 25% . . 12%
1	B	1260	2% 49% 32% 6% . 11%
1	C	1260	57% 26% . . 12%
1	D	1260	2% 56% 28% . . 11%
2	E	5	60% 40%

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Mol	Chain	Length	Quality of chain
3	F	3	 33%67%
3	H	3	 33%67%
4	G	4	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36079 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 UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1111	Total	C	N	O	S	0	0	0
			8882	5671	1509	1675	27			
1	B	1120	Total	C	N	O	S	0	0	0
			8955	5718	1522	1688	27			
1	C	1113	Total	C	N	O	S	0	0	0
			8898	5680	1512	1678	28			
1	D	1123	Total	C	N	O	S	0	0	0
			8983	5735	1529	1691	28			

There are 48 discrepancies between the modelled and reference sequences:

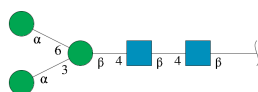
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58
B	21	GLU	-	expression tag	UNP G0SB58
B	22	THR	-	expression tag	UNP G0SB58
B	23	GLY	-	expression tag	UNP G0SB58
B	1506	GLY	-	expression tag	UNP G0SB58
B	1507	THR	-	expression tag	UNP G0SB58
B	1508	LYS	-	expression tag	UNP G0SB58
B	1509	HIS	-	expression tag	UNP G0SB58
B	1510	HIS	-	expression tag	UNP G0SB58

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1511	HIS	-	expression tag	UNP G0SB58
B	1512	HIS	-	expression tag	UNP G0SB58
B	1513	HIS	-	expression tag	UNP G0SB58
B	1514	HIS	-	expression tag	UNP G0SB58
C	21	GLU	-	expression tag	UNP G0SB58
C	22	THR	-	expression tag	UNP G0SB58
C	23	GLY	-	expression tag	UNP G0SB58
C	1506	GLY	-	expression tag	UNP G0SB58
C	1507	THR	-	expression tag	UNP G0SB58
C	1508	LYS	-	expression tag	UNP G0SB58
C	1509	HIS	-	expression tag	UNP G0SB58
C	1510	HIS	-	expression tag	UNP G0SB58
C	1511	HIS	-	expression tag	UNP G0SB58
C	1512	HIS	-	expression tag	UNP G0SB58
C	1513	HIS	-	expression tag	UNP G0SB58
C	1514	HIS	-	expression tag	UNP G0SB58
D	21	GLU	-	expression tag	UNP G0SB58
D	22	THR	-	expression tag	UNP G0SB58
D	23	GLY	-	expression tag	UNP G0SB58
D	1506	GLY	-	expression tag	UNP G0SB58
D	1507	THR	-	expression tag	UNP G0SB58
D	1508	LYS	-	expression tag	UNP G0SB58
D	1509	HIS	-	expression tag	UNP G0SB58
D	1510	HIS	-	expression tag	UNP G0SB58
D	1511	HIS	-	expression tag	UNP G0SB58
D	1512	HIS	-	expression tag	UNP G0SB58
D	1513	HIS	-	expression tag	UNP G0SB58
D	1514	HIS	-	expression tag	UNP G0SB58

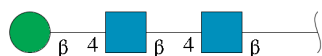
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



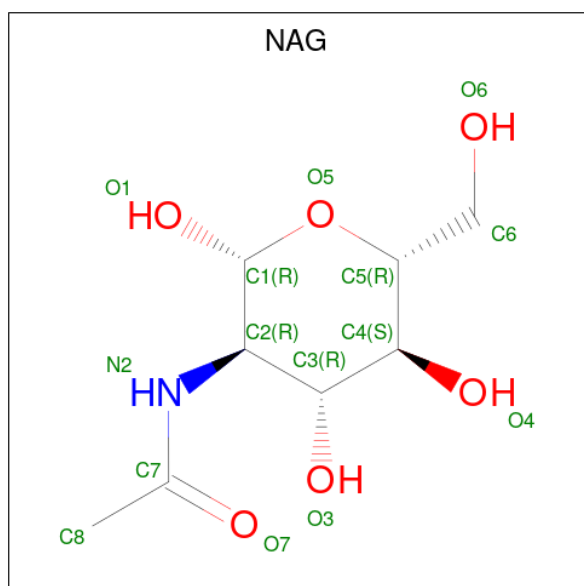
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

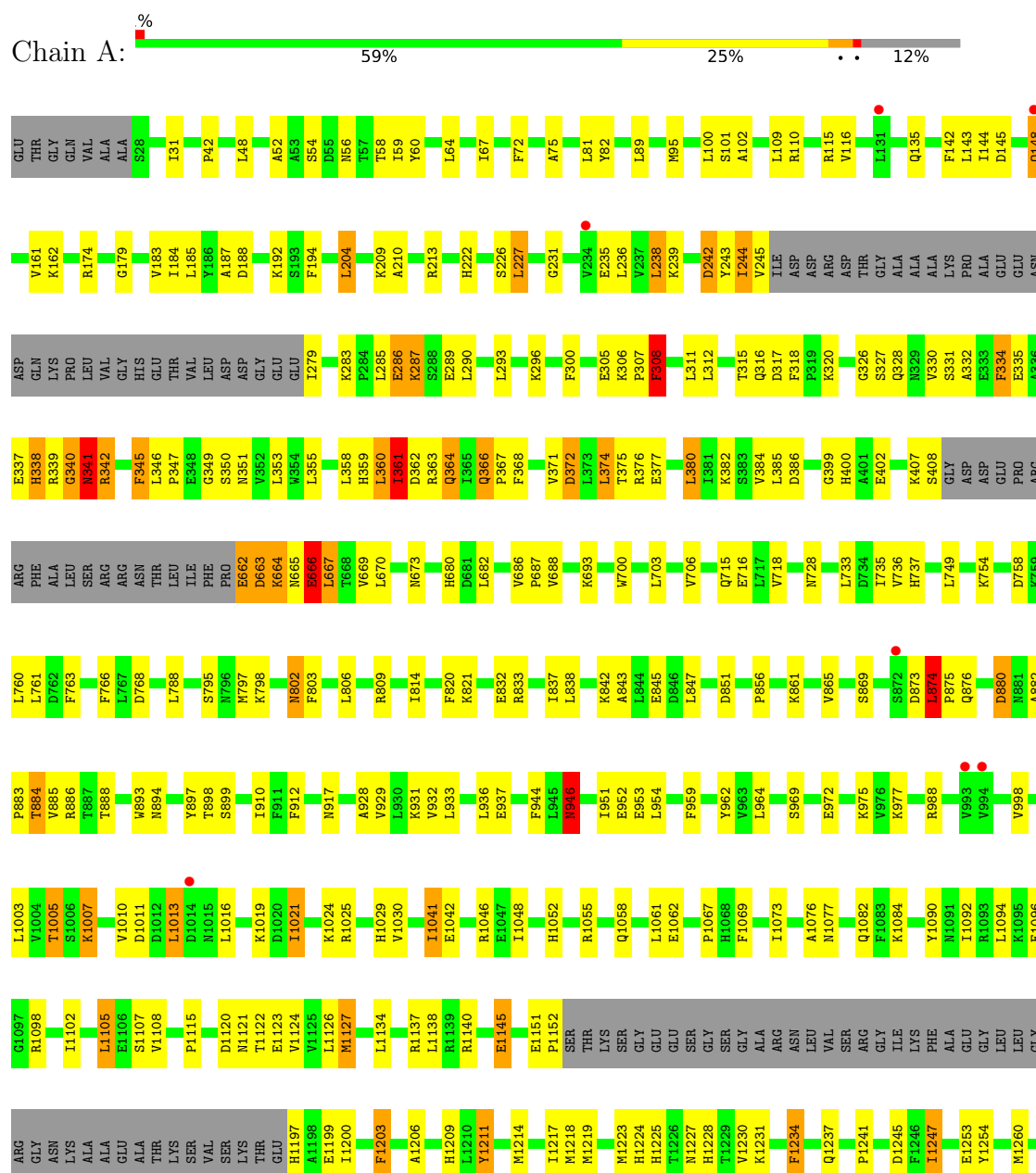
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

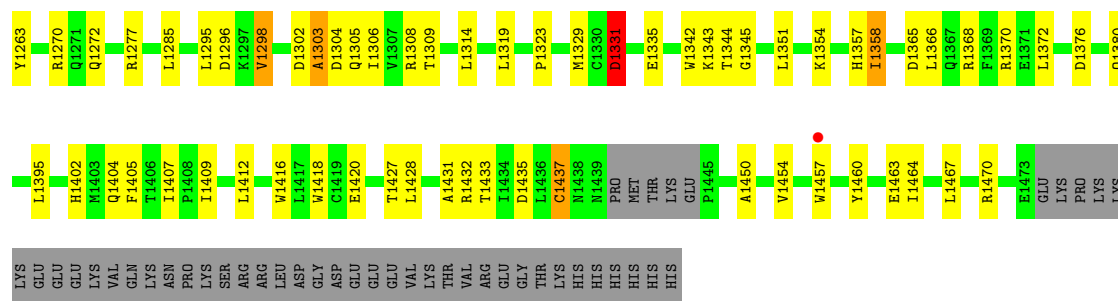
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0

3 Residue-property plots

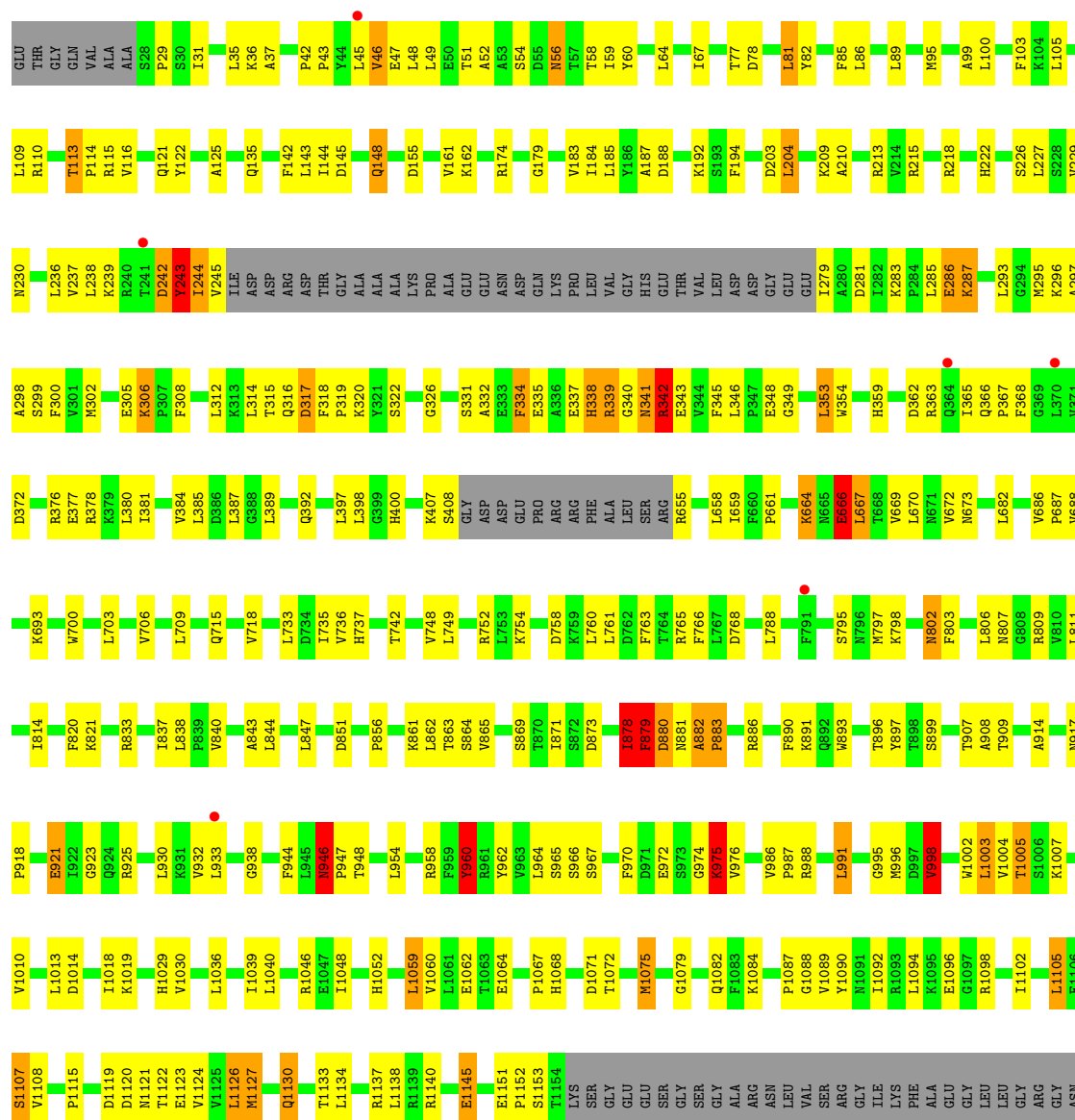
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

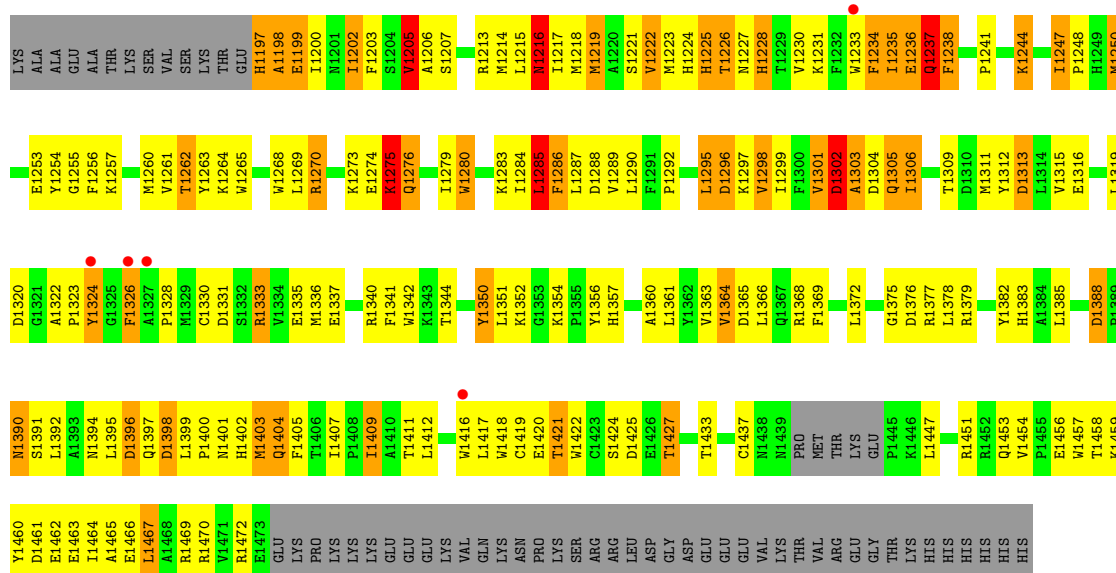
- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein





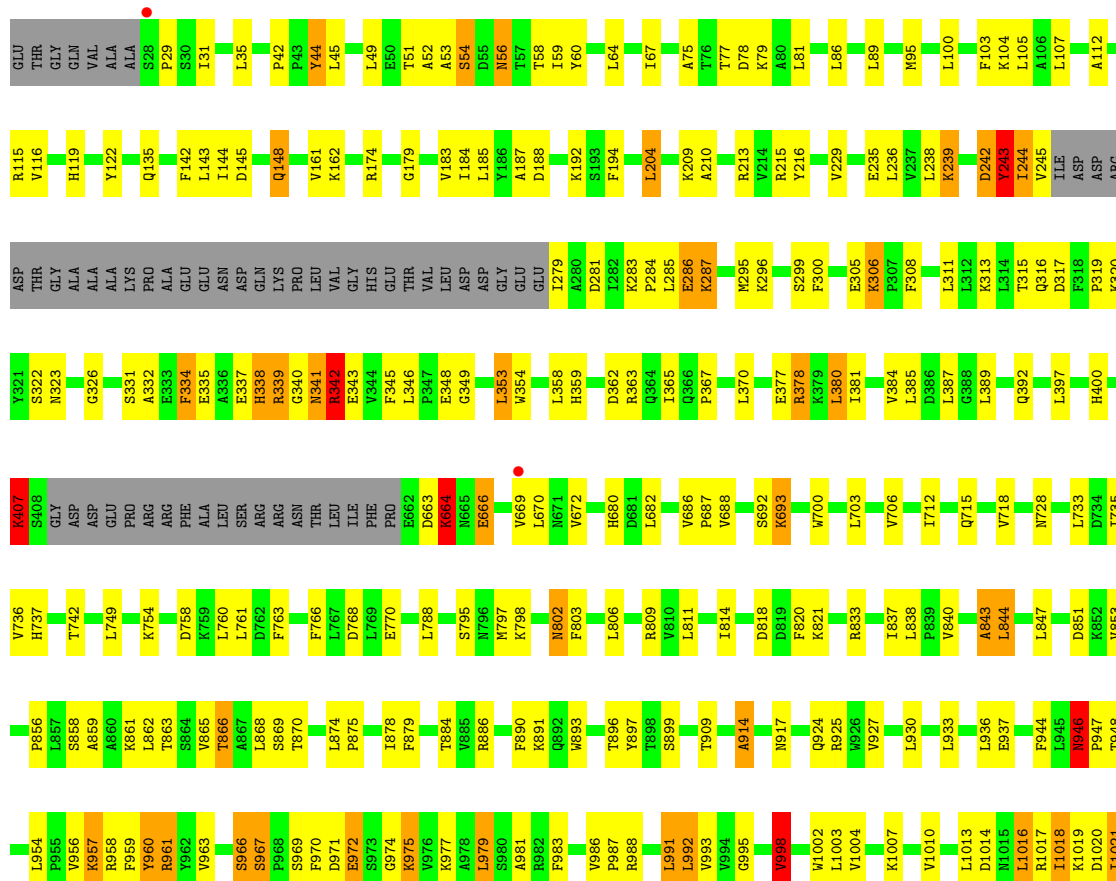
- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

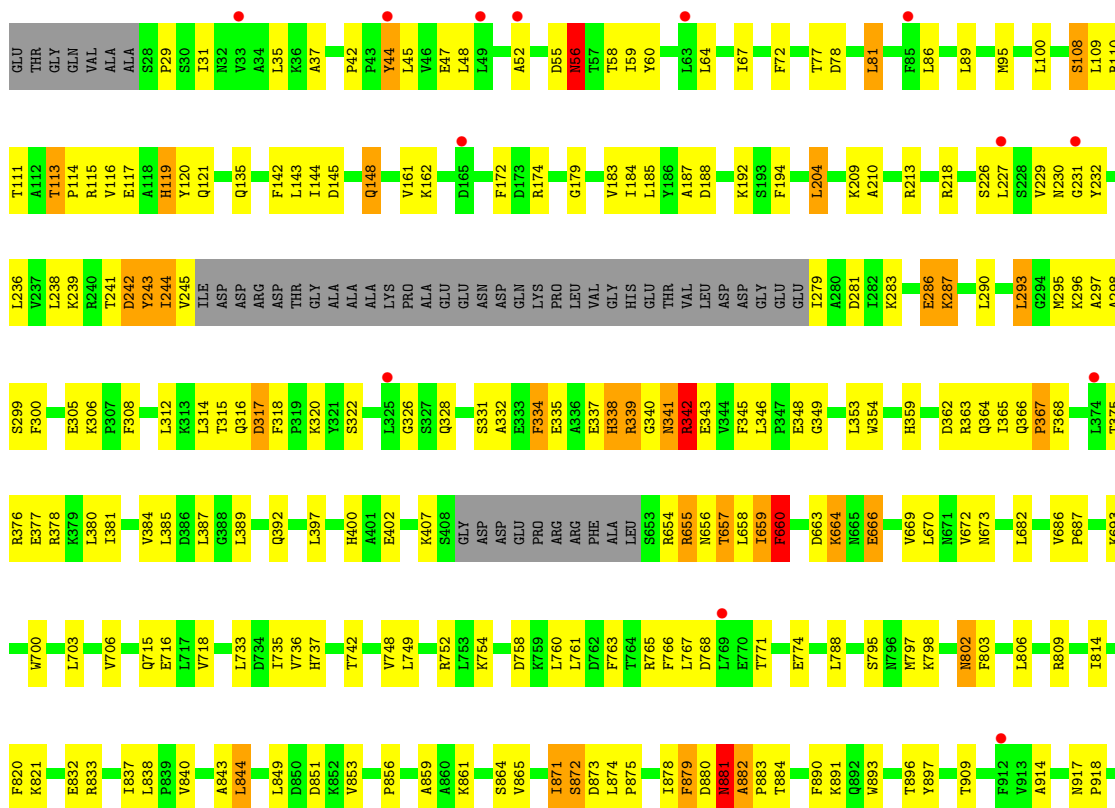
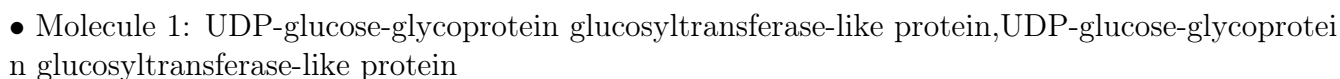


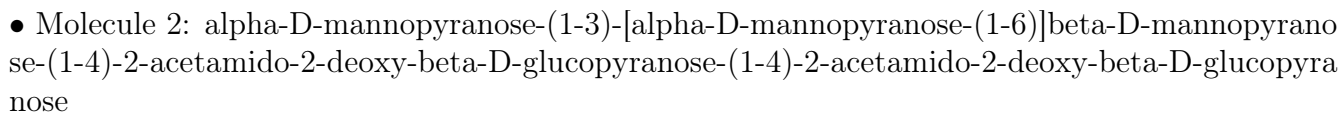


• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

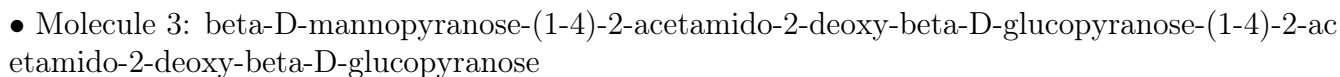
Chain C: 57% 26% 12%



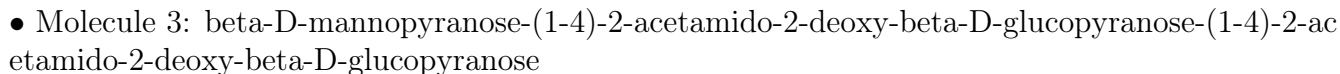




Opinion	Percentage
Doing a good job	60%
Doing a bad job	40%



Satisfaction Level	Percentage
Very satisfied	33%
Satisfied	67%



Opinion	Percentage
Doing a good job	33%
Doing a bad job	67%



Chain G:  100%

MAG1
MAG2
BGLA3
MAIN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.15Å 191.01Å 158.81Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	140.60 – 5.74 140.60 – 5.74	Depositor EDS
% Data completeness (in resolution range)	74.9 (140.60-5.74) 75.4 (140.60-5.74)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 5.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.249 0.184 , 0.253	Depositor DCC
R_{free} test set	829 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	290.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 466.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	36079	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: BMA, 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	0.79	8/9087 (0.1%)	1.22	48/12325 (0.4%)
1	B	0.83	5/9162 (0.1%)	1.27	79/12428 (0.6%)
1	C	0.79	7/9104 (0.1%)	1.20	43/12349 (0.3%)
1	D	0.78	3/9191 (0.0%)	1.23	53/12467 (0.4%)
All	All	0.80	23/36544 (0.1%)	1.23	223/49569 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	ASP	CA-C	7.28	1.62	1.52
1	C	666	GLU	CA-C	7.25	1.61	1.52
1	A	664	LYS	C-N	6.73	1.43	1.33
1	A	882	ALA	CA-C	6.57	1.61	1.52
1	A	665	ASN	CA-C	6.25	1.61	1.52
1	B	666	GLU	CA-C	6.24	1.59	1.52
1	A	663	ASP	C-N	6.20	1.41	1.33
1	C	1018	ILE	CA-C	6.19	1.60	1.52
1	B	873	ASP	CA-C	6.19	1.61	1.52
1	C	664	LYS	CA-C	6.14	1.60	1.52
1	C	1021	ILE	CA-C	5.94	1.60	1.52
1	C	663	ASP	C-N	5.88	1.40	1.33
1	C	1017	ARG	CA-C	5.81	1.60	1.52
1	B	659	ILE	CA-C	5.70	1.59	1.52
1	A	666	GLU	CA-C	5.62	1.60	1.52
1	B	1198	ALA	CA-C	5.57	1.59	1.52
1	D	655	ARG	CA-C	5.49	1.60	1.52
1	D	657	THR	CA-C	5.35	1.59	1.52
1	A	666	GLU	C-N	5.30	1.39	1.33
1	D	1439	ASN	CA-C	5.24	1.59	1.52
1	B	1275	LYS	CA-C	5.19	1.59	1.52
1	C	1439	ASN	CA-C	5.11	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	GLN	CA-C	5.03	1.59	1.52

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASN	CA-CB-CG	12.12	124.72	112.60
1	A	308	PHE	CA-CB-CG	9.60	123.39	113.80
1	D	881	ASN	CA-CB-CG	9.54	122.14	112.60
1	B	871	ILE	CA-C-N	8.32	136.68	121.70
1	B	871	ILE	C-N-CA	8.32	136.68	121.70
1	D	119	HIS	CA-C-N	8.16	131.88	120.29
1	D	119	HIS	C-N-CA	8.16	131.88	120.29
1	D	660	PHE	CA-CB-CG	-7.92	105.88	113.80
1	A	1245	ASP	CA-CB-CG	7.90	120.50	112.60
1	D	875	PRO	CA-C-N	7.87	135.87	121.70
1	D	875	PRO	C-N-CA	7.87	135.87	121.70
1	A	305	GLU	CA-C-N	7.81	131.44	122.85
1	A	305	GLU	C-N-CA	7.81	131.44	122.85
1	B	1302	ASP	CA-CB-CG	7.75	120.35	112.60
1	B	879	PHE	CA-CB-CG	7.73	121.53	113.80
1	D	1203	PHE	CA-CB-CG	7.54	121.34	113.80
1	D	946	ASN	CA-CB-CG	7.47	120.08	112.60
1	C	1203	PHE	CA-CB-CG	7.44	121.24	113.80
1	A	1203	PHE	CA-CB-CG	7.30	121.10	113.80
1	D	243	TYR	CA-C-N	7.26	135.04	121.97
1	D	243	TYR	C-N-CA	7.26	135.04	121.97
1	D	883	PRO	CA-C-N	7.22	131.12	120.87
1	D	883	PRO	C-N-CA	7.22	131.12	120.87
1	B	946	ASN	CA-CB-CG	7.18	119.78	112.60
1	B	1274	GLU	CA-C-N	6.93	134.77	121.54
1	B	1274	GLU	C-N-CA	6.93	134.77	121.54
1	A	345	PHE	CA-CB-CG	6.88	120.68	113.80
1	C	243	TYR	CA-C-N	6.88	134.35	121.97
1	C	243	TYR	C-N-CA	6.88	134.35	121.97
1	C	1020	ASP	CA-C-N	6.85	134.30	121.97
1	C	1020	ASP	C-N-CA	6.85	134.30	121.97
1	B	243	TYR	CA-C-N	6.85	134.30	121.97
1	B	243	TYR	C-N-CA	6.85	134.30	121.97
1	C	946	ASN	CA-CB-CG	6.83	119.42	112.60
1	B	1372	LEU	CA-C-N	6.76	132.00	122.46
1	B	1372	LEU	C-N-CA	6.76	132.00	122.46
1	C	305	GLU	CA-C-N	6.72	130.25	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	GLU	C-N-CA	6.72	130.25	122.85
1	D	1237	GLN	N-CA-C	6.58	118.11	111.07
1	D	960	TYR	N-CA-C	6.56	119.03	107.61
1	B	317	ASP	CA-C-N	6.49	127.83	119.78
1	B	317	ASP	C-N-CA	6.49	127.83	119.78
1	A	1234	PHE	CA-CB-CG	6.46	120.26	113.80
1	D	1234	PHE	CA-CB-CG	6.43	120.23	113.80
1	B	673	ASN	CA-C-N	6.40	129.68	120.79
1	B	673	ASN	C-N-CA	6.40	129.68	120.79
1	D	1238	PHE	CA-CB-CG	6.34	120.14	113.80
1	D	305	GLU	CA-C-N	6.29	129.77	122.85
1	D	305	GLU	C-N-CA	6.29	129.77	122.85
1	A	306	LYS	N-CA-C	-6.29	98.06	108.75
1	B	1216	ASN	CA-C-N	6.28	128.60	120.56
1	B	1216	ASN	C-N-CA	6.28	128.60	120.56
1	D	1302	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	1285	LEU	N-CA-C	6.24	118.16	111.36
1	D	659	ILE	N-CA-C	6.20	117.05	107.99
1	D	871	ILE	N-CA-CB	6.18	118.07	111.46
1	C	342	ARG	CA-C-N	6.14	129.12	120.28
1	C	342	ARG	C-N-CA	6.14	129.12	120.28
1	A	242	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	1224	HIS	CA-C-N	6.14	133.26	121.54
1	B	1224	HIS	C-N-CA	6.14	133.26	121.54
1	C	1302	ASP	CA-C-N	6.11	133.21	121.54
1	C	1302	ASP	C-N-CA	6.11	133.21	121.54
1	B	1227	ASN	CA-C-N	6.10	132.53	121.06
1	B	1227	ASN	C-N-CA	6.10	132.53	121.06
1	B	1304	ASP	CA-CB-CG	6.08	118.69	112.60
1	C	1302	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	1302	ASP	CA-C-N	6.03	133.06	121.54
1	D	1302	ASP	C-N-CA	6.03	133.06	121.54
1	B	879	PHE	CA-C-N	6.03	132.55	121.70
1	B	879	PHE	C-N-CA	6.03	132.55	121.70
1	C	306	LYS	N-CA-C	-6.01	98.54	108.75
1	C	1021	ILE	CA-C-N	6.01	130.85	120.58
1	C	1021	ILE	C-N-CA	6.01	130.85	120.58
1	B	47	GLU	N-CA-C	-6.00	104.66	111.14
1	A	1302	ASP	CA-C-N	5.99	132.98	121.54
1	A	1302	ASP	C-N-CA	5.99	132.98	121.54
1	C	1234	PHE	CA-CB-CG	5.99	119.79	113.80
1	D	1236	GLU	N-CA-C	5.98	118.29	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	960	TYR	N-CA-C	5.98	118.27	108.52
1	A	366	GLN	N-CA-C	-5.97	99.84	109.40
1	A	1016	LEU	N-CA-C	5.95	118.91	109.50
1	B	1222	VAL	N-CA-C	-5.95	105.05	110.82
1	B	1463	GLU	CA-C-N	5.93	128.84	120.42
1	B	1463	GLU	C-N-CA	5.93	128.84	120.42
1	D	300	PHE	CA-CB-CG	-5.93	107.87	113.80
1	A	1302	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	242	ASP	CA-CB-CG	5.91	118.50	112.60
1	B	1313	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	1288	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	386	ASP	CA-C-N	5.82	132.56	122.56
1	A	386	ASP	C-N-CA	5.82	132.56	122.56
1	A	340	GLY	CA-C-N	5.81	128.00	120.44
1	A	340	GLY	C-N-CA	5.81	128.00	120.44
1	D	242	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	1405	PHE	CA-CB-CG	5.77	119.57	113.80
1	D	1285	LEU	N-CA-C	5.75	117.35	111.14
1	B	51	THR	N-CA-C	-5.73	105.31	112.93
1	B	1205	VAL	CA-C-N	5.73	132.48	121.54
1	B	1205	VAL	C-N-CA	5.73	132.48	121.54
1	A	946	ASN	CA-CB-CG	5.71	118.31	112.60
1	B	306	LYS	N-CA-C	-5.70	99.06	108.75
1	D	306	LYS	N-CA-C	-5.69	99.07	108.75
1	B	878	ILE	N-CA-CB	5.69	116.59	110.62
1	B	305	GLU	CA-C-N	5.68	129.10	122.85
1	B	305	GLU	C-N-CA	5.68	129.10	122.85
1	A	880	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	1198	ALA	N-CA-C	5.66	117.44	108.79
1	A	998	VAL	N-CA-CB	-5.64	103.31	111.21
1	C	960	TYR	N-CA-C	5.64	118.63	108.48
1	A	1227	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	937	GLU	CB-CG-CD	5.62	122.15	112.60
1	C	1236	GLU	N-CA-C	5.59	119.85	113.19
1	B	1286	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	44	TYR	N-CA-C	5.59	117.45	111.36
1	A	843	ALA	CA-C-N	5.58	128.02	120.65
1	A	843	ALA	C-N-CA	5.58	128.02	120.65
1	B	300	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	328	GLN	CB-CG-CD	5.58	122.08	112.60
1	C	242	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	880	ASP	CA-C-N	5.57	131.73	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	880	ASP	C-N-CA	5.57	131.73	121.70
1	D	334	PHE	N-CA-C	-5.56	104.61	111.40
1	B	970	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	235	GLU	CB-CG-CD	5.55	122.04	112.60
1	B	1404	GLN	CA-C-N	5.55	128.50	120.79
1	B	1404	GLN	C-N-CA	5.55	128.50	120.79
1	A	334	PHE	N-CA-C	-5.54	104.64	111.40
1	C	1365	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	1041	ILE	N-CA-C	-5.54	98.48	107.28
1	C	843	ALA	CA-C-N	5.53	127.63	120.44
1	C	843	ALA	C-N-CA	5.53	127.63	120.44
1	A	1331	ASP	CA-C-N	5.52	128.14	120.63
1	A	1331	ASP	C-N-CA	5.52	128.14	120.63
1	A	364	GLN	N-CA-C	-5.52	106.31	113.16
1	D	342	ARG	CA-C-N	5.52	129.43	120.60
1	D	342	ARG	C-N-CA	5.52	129.43	120.60
1	A	327	SER	CA-C-N	5.52	130.79	122.68
1	A	327	SER	C-N-CA	5.52	130.79	122.68
1	B	1228	HIS	N-CA-C	5.50	117.17	110.41
1	D	59	ILE	CA-C-N	5.49	127.95	120.54
1	D	59	ILE	C-N-CA	5.49	127.95	120.54
1	B	923	GLY	CA-C-N	5.45	127.85	120.38
1	B	923	GLY	C-N-CA	5.45	127.85	120.38
1	D	1331	ASP	CA-C-N	5.45	128.04	120.63
1	D	1331	ASP	C-N-CA	5.45	128.04	120.63
1	D	188	ASP	N-CA-C	-5.44	97.64	107.75
1	C	59	ILE	CA-C-N	5.43	127.87	120.54
1	C	59	ILE	C-N-CA	5.43	127.87	120.54
1	B	1292	PRO	CA-C-N	5.42	127.81	120.38
1	B	1292	PRO	C-N-CA	5.42	127.81	120.38
1	C	188	ASP	N-CA-C	-5.41	97.69	107.75
1	C	334	PHE	N-CA-C	-5.41	104.80	111.40
1	D	914	ALA	N-CA-C	5.40	117.54	108.96
1	B	334	PHE	N-CA-C	-5.39	104.82	111.40
1	A	59	ILE	CA-C-N	5.39	127.81	120.54
1	A	59	ILE	C-N-CA	5.39	127.81	120.54
1	B	1341	PHE	CA-CB-CG	5.37	119.17	113.80
1	B	59	ILE	CA-C-N	5.36	127.77	120.54
1	B	59	ILE	C-N-CA	5.36	127.77	120.54
1	C	998	VAL	CB-CA-C	5.36	116.67	110.89
1	B	908	ALA	N-CA-C	5.35	117.83	108.52
1	A	188	ASP	N-CA-C	-5.34	97.82	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	728	ASN	CA-C-N	5.31	127.39	120.28
1	A	728	ASN	C-N-CA	5.31	127.39	120.28
1	B	1234	PHE	CA-CB-CG	5.30	119.10	113.80
1	D	108	SER	CA-C-N	5.30	127.39	120.28
1	D	108	SER	C-N-CA	5.30	127.39	120.28
1	C	992	LEU	CA-C-N	5.29	131.50	121.97
1	C	992	LEU	C-N-CA	5.29	131.50	121.97
1	C	728	ASN	CA-C-N	5.29	127.37	120.28
1	C	728	ASN	C-N-CA	5.29	127.37	120.28
1	D	317	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	1014	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	342	ARG	CA-C-N	5.27	129.03	120.60
1	B	342	ARG	C-N-CA	5.27	129.03	120.60
1	D	1236	GLU	CA-C-N	5.27	127.29	120.44
1	D	1236	GLU	C-N-CA	5.27	127.29	120.44
1	C	300	PHE	CA-CB-CG	-5.26	108.54	113.80
1	B	1088	GLY	N-CA-C	5.25	117.67	110.69
1	B	188	ASP	N-CA-C	-5.25	97.99	107.75
1	C	914	ALA	N-CA-C	5.25	117.25	108.23
1	B	187	ALA	N-CA-C	5.24	117.77	109.50
1	B	203	ASP	CA-CB-CG	5.22	117.82	112.60
1	D	879	PHE	CA-C-N	5.20	131.48	121.54
1	D	879	PHE	C-N-CA	5.20	131.48	121.54
1	C	1331	ASP	CA-C-N	5.20	127.70	120.63
1	C	1331	ASP	C-N-CA	5.20	127.70	120.63
1	A	72	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	187	ALA	N-CA-C	5.19	117.70	109.50
1	B	1350	TYR	N-CA-C	-5.18	106.04	112.93
1	D	56	ASN	CA-C-N	5.18	127.22	120.28
1	D	56	ASN	C-N-CA	5.18	127.22	120.28
1	D	655	ARG	CA-C-N	5.17	131.41	121.54
1	D	655	ARG	C-N-CA	5.17	131.41	121.54
1	D	187	ALA	N-CA-C	5.13	117.61	109.50
1	C	866	THR	N-CA-C	5.13	116.56	110.97
1	B	1462	GLU	CA-C-N	5.13	127.41	120.44
1	B	1462	GLU	C-N-CA	5.13	127.41	120.44
1	B	998	VAL	CB-CA-C	5.13	116.43	110.89
1	B	962	TYR	N-CA-C	5.12	117.06	107.99
1	D	318	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	187	ALA	N-CA-C	5.11	117.57	109.50
1	C	1275	LYS	CA-C-N	5.09	127.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1275	LYS	C-N-CA	5.09	127.06	120.44
1	B	1326	PHE	CA-CB-CG	5.09	118.89	113.80
1	D	1243	PHE	CA-C-N	5.06	127.06	120.28
1	D	1243	PHE	C-N-CA	5.06	127.06	120.28
1	A	347	PRO	N-CA-C	5.05	119.16	111.34
1	C	56	ASN	CA-C-N	5.03	127.03	120.28
1	C	56	ASN	C-N-CA	5.03	127.03	120.28
1	B	921	GLU	CA-C-N	5.03	127.93	120.74
1	B	921	GLU	C-N-CA	5.03	127.93	120.74
1	B	1227	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	667	LEU	N-CA-C	5.02	116.06	108.07
1	B	1302	ASP	CA-C-N	5.02	131.12	121.54
1	B	1302	ASP	C-N-CA	5.02	131.12	121.54
1	B	667	LEU	CA-C-N	5.01	129.70	121.58
1	B	667	LEU	C-N-CA	5.01	129.70	121.58
1	A	361	ILE	CA-C-N	5.00	127.30	120.54
1	A	361	ILE	C-N-CA	5.00	127.30	120.54
1	A	1358	ILE	N-CA-C	5.00	115.06	107.75

There are no chirality outliers.

There are no planarity outliers.

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	8882	0	8770	234	0
1	B	8955	0	8846	337	0
1	C	8898	0	8788	282	0
1	D	8983	0	8881	293	0
2	E	61	0	52	4	0
3	F	39	0	34	0	0
3	H	39	0	34	0	0
4	G	50	0	43	0	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
5	C	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	42	0	39	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	36079	0	35604	1116	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 16.

All (1116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ASP:HB2	1:D:975:LYS:HA	1.23	1.16
1:B:1376:ASP:HA	1:B:1379:ARG:HD3	1.26	1.15
1:B:1333:ARG:HG3	1:B:1424:SER:HA	1.17	1.13
1:D:1241:PRO:HA	1:D:1244:LYS:HB2	1.32	1.12
1:B:869:SER:HB2	1:B:886:ARG:HE	1.07	1.10
1:D:364:GLN:HG2	1:D:880:ASP:HB2	1.32	1.10
1:B:921:GLU:HB3	1:B:958:ARG:HE	1.03	1.09
1:B:1107:SER:HB2	1:B:1120:ASP:HA	1.35	1.08
1:D:42:PRO:HB3	1:D:116:VAL:HG11	1.31	1.07
1:D:1107:SER:HB2	1:D:1120:ASP:HA	1.38	1.04
1:A:673:ASN:HA	1:A:861:LYS:HE2	1.39	1.04
1:C:1107:SER:HB2	1:C:1120:ASP:HA	1.36	1.03
1:A:243:TYR:HB3	1:A:285:LEU:HG	1.41	1.03
1:A:1107:SER:HB2	1:A:1120:ASP:HA	1.39	1.01
1:A:1270:ARG:HH12	1:C:821:LYS:NZ	1.57	1.00
1:A:296:LYS:HD2	1:A:326:GLY:HA2	1.43	1.00
1:A:874:LEU:H	1:A:875:PRO:HA	1.27	1.00
1:A:1105:LEU:HA	1:A:1138:LEU:HG	1.44	0.99
1:D:1367:GLN:HE22	1:D:1370:ARG:HH11	1.05	0.99
1:B:1202:ILE:HG12	1:B:1299:ILE:HB	1.44	0.98
1:B:1105:LEU:HA	1:B:1138:LEU:HG	1.43	0.98
1:B:1404:GLN:HG3	1:B:1409:ILE:HB	1.46	0.97
1:D:1105:LEU:HA	1:D:1138:LEU:HG	1.47	0.97
1:D:1439:ASN:HB3	1:D:1440:PRO:HA	1.47	0.97
1:B:1197:HIS:N	1:B:1257:LYS:HZ3	1.63	0.96
1:C:1439:ASN:HB3	1:C:1440:PRO:HA	1.47	0.96
1:C:1105:LEU:HA	1:C:1138:LEU:HG	1.46	0.96
1:D:387:LEU:HD21	1:D:861:LYS:HB2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:NH2	1:D:174:ARG:HH21	1.62	0.95
1:B:1466:GLU:HA	1:B:1469:ARG:HD2	1.46	0.94
1:A:1270:ARG:HH12	1:C:821:LYS:HZ1	1.05	0.94
1:B:869:SER:HB2	1:B:886:ARG:NE	1.83	0.93
1:B:1357:HIS:NE2	1:B:1411:THR:HG22	1.82	0.93
1:C:878:ILE:HG23	1:C:1044:HIS:HE1	1.32	0.93
1:B:1270:ARG:HH12	1:D:821:LYS:NZ	1.66	0.92
1:B:921:GLU:HB3	1:B:958:ARG:NE	1.84	0.91
1:C:878:ILE:HG23	1:C:1044:HIS:CE1	2.07	0.90
1:D:1416:TRP:HA	1:D:1432:ARG:HB2	1.53	0.90
1:A:802:ASN:HB2	1:A:814:ILE:HB	1.53	0.89
1:B:802:ASN:HB2	1:B:814:ILE:HB	1.52	0.89
1:B:1340:ARG:HE	1:B:1422:TRP:HD1	1.19	0.89
1:B:78:ASP:HB2	1:B:975:LYS:HA	1.54	0.89
1:D:672:VAL:HB	1:D:861:LYS:HA	1.52	0.89
1:D:1367:GLN:NE2	1:D:1370:ARG:HH11	1.69	0.89
1:B:1302:ASP:OD1	1:B:1302:ASP:O	1.90	0.88
1:A:1098:ARG:HE	1:A:1152:PRO:HD3	1.40	0.87
1:D:77:THR:HB	1:D:974:GLY:HA3	1.55	0.87
1:C:802:ASN:HB2	1:C:814:ILE:HB	1.55	0.87
1:D:802:ASN:HB2	1:D:814:ILE:HB	1.54	0.86
1:C:858:SER:HA	1:C:861:LYS:HE2	1.58	0.86
1:C:1214:MET:HE3	1:C:1457:TRP:HE1	1.39	0.86
1:C:1416:TRP:HA	1:C:1432:ARG:HB2	1.57	0.85
1:A:1214:MET:HE3	1:A:1457:TRP:HE1	1.39	0.85
1:D:673:ASN:HA	1:D:861:LYS:HD2	1.57	0.85
1:B:880:ASP:HB3	1:B:881:ASN:HA	1.57	0.84
1:C:79:LYS:NZ	1:C:972:GLU:HA	1.92	0.84
1:A:1416:TRP:HA	1:A:1432:ARG:HB2	1.57	0.84
1:D:1214:MET:HE3	1:D:1457:TRP:HE1	1.41	0.84
1:B:349:GLY:HA3	1:B:948:THR:HB	1.60	0.84
1:B:155:ASP:OD1	1:C:1142:PRO:HG3	1.78	0.83
1:B:879:PHE:HB2	1:B:880:ASP:HA	1.60	0.83
1:C:79:LYS:HE3	1:C:970:PHE:HB3	1.60	0.83
1:B:1270:ARG:HH12	1:D:821:LYS:HZ3	1.22	0.82
1:C:105:LEU:HG	1:C:966:SER:HA	1.61	0.82
1:A:1062:GLU:HB2	1:A:1067:PRO:HA	1.61	0.82
1:B:1062:GLU:HB2	1:B:1067:PRO:HA	1.62	0.82
1:D:117:GLU:HA	1:D:120:TYR:HB2	1.60	0.82
1:B:1270:ARG:NH1	1:D:821:LYS:NZ	2.27	0.82
2:E:1:NAG:H61	2:E:2:NAG:N2	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LYS:HD3	1:B:326:GLY:HA2	1.62	0.81
1:C:349:GLY:HA3	1:C:948:THR:HB	1.62	0.81
1:B:1276:GLN:HA	1:B:1279:ILE:HB	1.60	0.81
1:B:1469:ARG:HA	1:B:1472:ARG:HD2	1.63	0.81
1:C:1197:HIS:HE1	1:C:1231:LYS:HZ2	1.29	0.81
1:B:77:THR:HB	1:B:974:GLY:HA3	1.62	0.80
1:C:296:LYS:HD3	1:C:326:GLY:HA2	1.64	0.80
1:A:1214:MET:HE3	1:A:1457:TRP:NE1	1.96	0.80
1:D:339:ARG:HH12	1:D:946:ASN:HB2	1.46	0.80
1:A:345:PHE:HB3	1:A:893:TRP:HE1	1.46	0.80
1:D:1062:GLU:HB2	1:D:1067:PRO:HA	1.62	0.80
1:B:338:HIS:CD2	1:B:341:ASN:HD21	2.00	0.80
1:D:349:GLY:HA3	1:D:948:THR:HB	1.63	0.80
1:C:77:THR:HB	1:C:974:GLY:HA3	1.64	0.79
1:B:245:VAL:HB	1:B:287:LYS:HA	1.63	0.79
1:C:245:VAL:HB	1:C:287:LYS:HA	1.65	0.79
1:C:1062:GLU:HB2	1:C:1067:PRO:HA	1.63	0.79
1:C:1214:MET:HE3	1:C:1457:TRP:NE1	1.97	0.79
1:C:338:HIS:CD2	1:C:341:ASN:HD21	2.00	0.79
1:B:1382:TYR:HA	1:B:1385:LEU:HG	1.64	0.79
1:A:296:LYS:HE2	1:A:331:SER:HA	1.64	0.78
1:C:693:LYS:NZ	1:C:693:LYS:H	1.80	0.78
1:B:1333:ARG:HG3	1:B:1424:SER:CA	2.07	0.78
1:C:692:SER:HA	1:C:693:LYS:NZ	1.97	0.78
1:D:338:HIS:CD2	1:D:341:ASN:HD21	2.01	0.78
1:C:339:ARG:HH12	1:C:946:ASN:HB2	1.49	0.78
1:A:1418:TRP:NE1	1:A:1427:THR:HB	1.99	0.78
1:B:339:ARG:HH12	1:B:946:ASN:HB2	1.48	0.77
1:D:1418:TRP:NE1	1:D:1427:THR:HB	1.98	0.77
1:A:821:LYS:NZ	1:C:1270:ARG:HH12	1.82	0.77
1:C:1418:TRP:NE1	1:C:1427:THR:HB	1.99	0.77
1:D:296:LYS:HD3	1:D:326:GLY:HA2	1.67	0.77
1:D:1214:MET:HE3	1:D:1457:TRP:NE1	1.99	0.77
1:B:239:LYS:HZ1	1:B:1275:LYS:HZ1	1.33	0.76
1:D:1418:TRP:HE1	1:D:1427:THR:HB	1.51	0.76
1:A:179:GLY:HA3	1:A:210:ALA:HA	1.68	0.76
1:B:1323:PRO:HB3	1:B:1369:PHE:HA	1.68	0.76
1:B:1197:HIS:N	1:B:1257:LYS:NZ	2.34	0.76
1:B:1340:ARG:HE	1:B:1422:TRP:CD1	2.04	0.76
1:A:1270:ARG:NH1	1:C:821:LYS:HZ1	1.81	0.76
1:A:842:LYS:HA	1:A:845:GLU:HG2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.51	0.76
1:D:296:LYS:HZ3	1:D:326:GLY:HA2	1.50	0.75
1:D:245:VAL:HB	1:D:287:LYS:HA	1.68	0.75
1:A:1197:HIS:HE1	1:A:1231:LYS:HZ2	1.34	0.75
1:B:1451:ARG:HE	1:B:1457:TRP:HH2	1.32	0.75
1:C:1253:GLU:HG3	1:C:1467:LEU:HD11	1.68	0.75
1:C:179:GLY:HA3	1:C:210:ALA:HA	1.69	0.75
1:B:49:LEU:HD21	1:B:64:LEU:HD13	1.67	0.74
1:B:1280:TRP:CD1	1:B:1283:LYS:HZ3	2.05	0.74
1:A:296:LYS:CD	1:A:326:GLY:HA2	2.18	0.74
1:C:338:HIS:CE1	1:C:896:THR:HB	2.23	0.74
1:D:1418:TRP:CD1	1:D:1427:THR:HB	2.21	0.74
1:C:79:LYS:HZ2	1:C:972:GLU:HA	1.51	0.74
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.52	0.74
1:D:1331:ASP:HB3	1:D:1343:LYS:HZ1	1.53	0.73
1:B:1402:HIS:NE2	1:D:767:LEU:HD13	2.02	0.73
1:B:179:GLY:HA3	1:B:210:ALA:HA	1.68	0.73
1:D:78:ASP:CB	1:D:975:LYS:HA	2.12	0.73
1:D:179:GLY:HA3	1:D:210:ALA:HA	1.69	0.73
1:D:1367:GLN:HE22	1:D:1370:ARG:NH1	1.86	0.73
1:C:1418:TRP:HE1	1:C:1427:THR:HB	1.51	0.73
1:D:338:HIS:CE1	1:D:896:THR:HB	2.24	0.73
1:B:1467:LEU:HD13	1:B:1470:ARG:HE	1.54	0.73
1:C:1306:ILE:HD11	1:C:1457:TRP:HD1	1.53	0.73
1:C:380:LEU:HD11	1:C:869:SER:HA	1.70	0.73
1:A:1253:GLU:HG3	1:A:1467:LEU:HD11	1.71	0.72
1:B:1202:ILE:CG1	1:B:1299:ILE:HB	2.19	0.72
1:A:1418:TRP:CD1	1:A:1427:THR:HB	2.24	0.72
1:C:1418:TRP:CD1	1:C:1427:THR:HB	2.24	0.72
1:A:969:SER:HB2	1:A:977:LYS:HB3	1.70	0.72
1:B:1460:TYR:O	1:B:1464:ILE:HG12	1.88	0.72
1:B:338:HIS:CE1	1:B:896:THR:HB	2.25	0.72
1:A:399:GLY:O	1:A:888:THR:HB	1.90	0.72
1:C:135:GLN:HE22	1:C:148:GLN:NE2	1.88	0.71
1:D:1354:LYS:HZ3	1:D:1405:PHE:HD1	1.36	0.71
1:D:95:MET:HB3	1:D:100:LEU:HG	1.72	0.71
1:D:335:GLU:HA	1:D:338:HIS:HB2	1.71	0.71
1:D:873:ASP:HB3	1:D:874:LEU:HA	1.73	0.71
1:D:296:LYS:NZ	1:D:326:GLY:HA2	2.05	0.71
1:A:1354:LYS:HZ3	1:A:1405:PHE:HD1	1.38	0.71
1:D:1253:GLU:HG3	1:D:1467:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:NZ	1:B:1275:LYS:NZ	2.38	0.71
1:B:335:GLU:HA	1:B:338:HIS:HB2	1.71	0.71
1:D:1306:ILE:HD11	1:D:1457:TRP:HD1	1.55	0.71
1:B:52:ALA:HB1	1:B:89:LEU:HD21	1.73	0.71
1:C:335:GLU:HA	1:C:338:HIS:HB2	1.72	0.71
1:D:961:ARG:NE	1:D:983:PHE:HA	2.05	0.70
1:C:1306:ILE:HG21	1:C:1454:VAL:HG11	1.71	0.70
1:D:115:ARG:HG2	1:D:1127:MET:HB2	1.73	0.70
1:B:1284:ILE:O	1:B:1285:LEU:HB2	1.91	0.70
1:A:236:LEU:HB2	1:A:959:PHE:HB2	1.74	0.70
1:D:44:TYR:HE2	1:D:110:ARG:NH2	1.88	0.70
1:C:358:LEU:HD22	1:C:884:THR:HG22	1.73	0.69
1:C:296:LYS:HE2	1:C:331:SER:HA	1.74	0.69
1:D:872:SER:HA	1:D:878:ILE:HB	1.73	0.69
1:D:342:ARG:HG2	1:D:346:LEU:O	1.93	0.69
1:D:135:GLN:HE22	1:D:148:GLN:NE2	1.91	0.69
1:B:1299:ILE:HD11	1:B:1315:VAL:HG22	1.73	0.69
1:C:35:LEU:HD23	1:C:229:VAL:HG23	1.74	0.69
1:D:1197:HIS:HE1	1:D:1231:LYS:NZ	1.91	0.69
1:B:135:GLN:HE22	1:B:148:GLN:NE2	1.89	0.69
1:C:1331:ASP:HB3	1:C:1343:LYS:HZ1	1.55	0.69
1:A:135:GLN:HE22	1:A:148:GLN:NE2	1.91	0.69
1:A:374:LEU:HG	1:A:375:THR:N	2.08	0.69
1:A:1306:ILE:HG21	1:A:1454:VAL:HG11	1.75	0.69
1:B:342:ARG:HG2	1:B:346:LEU:O	1.93	0.69
1:C:387:LEU:HD21	1:C:861:LYS:HB2	1.75	0.69
1:B:1298:VAL:HG12	1:B:1364:VAL:HG13	1.73	0.68
1:C:1060:VAL:HG22	1:C:1071:ASP:HB3	1.75	0.68
1:B:1385:LEU:HD22	1:B:1392:LEU:HD12	1.75	0.68
1:C:342:ARG:HG2	1:C:346:LEU:O	1.93	0.68
1:C:296:LYS:HZ3	1:C:326:GLY:HA2	1.58	0.68
1:D:1060:VAL:HG22	1:D:1071:ASP:HB3	1.75	0.68
1:A:874:LEU:N	1:A:875:PRO:HA	2.07	0.68
1:B:296:LYS:HE2	1:B:331:SER:HA	1.74	0.68
1:D:1306:ILE:HG21	1:D:1454:VAL:HG11	1.74	0.68
1:A:1331:ASP:HB3	1:A:1343:LYS:HZ1	1.59	0.68
1:A:821:LYS:HZ1	1:C:1270:ARG:HH12	1.39	0.68
1:B:239:LYS:NZ	1:B:1275:LYS:HZ1	1.91	0.68
1:D:115:ARG:HH22	1:D:174:ARG:HH21	1.41	0.67
1:A:243:TYR:O	1:A:244:ILE:HG13	1.94	0.67
1:D:296:LYS:HE2	1:D:331:SER:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.77	0.67
1:B:998:VAL:HG13	1:B:1002:TRP:HB2	1.76	0.67
1:B:1265:TRP:CE2	1:B:1269:LEU:HD23	2.29	0.67
1:D:844:LEU:HD12	1:D:849:LEU:HB2	1.77	0.67
1:B:1060:VAL:HG22	1:B:1071:ASP:HB3	1.75	0.67
1:B:1270:ARG:NH1	1:D:821:LYS:HZ1	1.91	0.67
1:D:364:GLN:CG	1:D:880:ASP:HB2	2.17	0.67
1:C:296:LYS:NZ	1:C:326:GLY:HA2	2.08	0.67
1:D:1197:HIS:HE1	1:D:1231:LYS:HZ2	1.41	0.67
1:C:1439:ASN:HB3	1:C:1440:PRO:CA	2.25	0.66
1:B:1203:PHE:HB2	1:B:1233:TRP:O	1.96	0.66
1:B:1324:TYR:HB3	1:B:1364:VAL:HB	1.78	0.66
1:C:1197:HIS:HE1	1:C:1231:LYS:NZ	1.93	0.66
1:D:334:PHE:O	1:D:337:GLU:HG2	1.95	0.66
1:B:1376:ASP:HA	1:B:1379:ARG:CD	2.17	0.66
1:D:1236:GLU:HG2	1:D:1244:LYS:HZ1	1.60	0.66
1:A:75:ALA:HB1	1:A:81:LEU:HB2	1.78	0.66
1:B:1467:LEU:HD13	1:B:1470:ARG:NE	2.11	0.65
1:B:1383:HIS:HD2	1:D:716:GLU:OE1	1.79	0.65
1:A:345:PHE:CB	1:A:893:TRP:HE1	2.08	0.65
1:A:1270:ARG:NH1	1:C:821:LYS:NZ	2.39	0.65
1:D:238:LEU:HD13	1:D:283:LYS:HD3	1.79	0.65
1:B:239:LYS:HZ1	1:B:1275:LYS:NZ	1.95	0.65
1:B:1270:ARG:CZ	1:D:821:LYS:HZ1	2.09	0.65
1:C:693:LYS:H	1:C:693:LYS:HZ3	1.43	0.65
1:B:238:LEU:HD13	1:B:283:LYS:HD3	1.78	0.65
1:B:334:PHE:O	1:B:337:GLU:HG2	1.97	0.65
1:D:999:PRO:HB2	1:D:1002:TRP:CD1	2.32	0.65
1:A:1197:HIS:HE1	1:A:1231:LYS:NZ	1.95	0.65
1:C:52:ALA:HB1	1:C:89:LEU:HD21	1.78	0.65
1:C:998:VAL:HG13	1:C:1002:TRP:HB2	1.79	0.65
1:C:319:PRO:HA	1:C:322:SER:HB2	1.79	0.65
1:B:296:LYS:NZ	1:B:326:GLY:HA2	2.12	0.65
1:A:1354:LYS:HD2	1:A:1404:GLN:HG3	1.79	0.64
1:B:672:VAL:HB	1:B:861:LYS:HA	1.78	0.64
1:B:1218:MET:HG3	1:B:1301:VAL:HG11	1.79	0.64
1:A:382:LYS:HA	1:A:385:LEU:HG	1.79	0.64
1:A:399:GLY:HA2	1:A:886:ARG:HB3	1.79	0.64
1:D:241:THR:HG21	1:D:957:LYS:HE2	1.79	0.64
1:A:300:PHE:CD2	1:A:330:VAL:HG21	2.32	0.64
1:B:1107:SER:CB	1:B:1120:ASP:HA	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:NAG:H61	2:E:2:NAG:HN2	1.60	0.64
1:B:1218:MET:HE2	1:B:1222:VAL:HG21	1.78	0.64
1:D:397:LEU:HD11	1:D:840:VAL:HG13	1.80	0.64
1:C:317:ASP:HB3	1:C:320:LYS:HB3	1.78	0.64
1:C:334:PHE:O	1:C:337:GLU:HG2	1.98	0.64
1:B:821:LYS:NZ	1:D:1270:ARG:HH12	1.97	0.63
1:B:1241:PRO:HA	1:B:1244:LYS:HB2	1.79	0.63
1:B:35:LEU:HD23	1:B:229:VAL:HG23	1.80	0.63
1:C:1329:MET:HG2	1:C:1358:ILE:HD11	1.81	0.63
1:A:1450:ALA:HB1	1:A:1457:TRP:CD2	2.34	0.63
1:D:1207:SER:CB	1:D:1279:ILE:HD11	2.29	0.63
1:A:238:LEU:HD13	1:A:283:LYS:HD3	1.81	0.63
1:B:1333:ARG:CG	1:B:1424:SER:HA	2.11	0.63
1:C:1354:LYS:HD2	1:C:1404:GLN:HG3	1.79	0.63
1:B:1465:ALA:HB1	1:B:1469:ARG:HH21	1.64	0.63
1:D:387:LEU:HD21	1:D:861:LYS:CB	2.25	0.63
1:D:1272:GLN:HB3	1:D:1277:ARG:HB2	1.80	0.62
1:D:1354:LYS:HD2	1:D:1404:GLN:HG3	1.81	0.62
1:A:346:LEU:HG	1:A:893:TRP:HZ2	1.64	0.62
1:C:238:LEU:HD13	1:C:283:LYS:HD3	1.81	0.62
1:C:833:ARG:HA	1:C:837:ILE:HB	1.81	0.62
1:C:316:GLN:HB2	1:C:961:ARG:CD	2.29	0.62
1:D:1439:ASN:HB3	1:D:1440:PRO:CA	2.25	0.62
1:B:400:HIS:CD2	1:B:843:ALA:HB2	2.33	0.62
1:B:1454:VAL:CG1	1:B:1456:GLU:HG2	2.30	0.62
1:B:95:MET:HB3	1:B:100:LEU:HG	1.82	0.62
1:B:833:ARG:HA	1:B:837:ILE:HB	1.82	0.62
1:D:963:VAL:HG22	1:D:981:ALA:HB2	1.80	0.62
1:D:1329:MET:HG2	1:D:1358:ILE:HD11	1.81	0.62
1:A:339:ARG:HD3	1:A:342:ARG:HB2	1.82	0.62
1:C:400:HIS:CD2	1:C:843:ALA:HB2	2.35	0.62
1:C:1234:PHE:HD1	1:C:1260:MET:SD	2.22	0.62
1:D:1107:SER:CB	1:D:1120:ASP:HA	2.24	0.62
1:B:1237:GLN:NE2	1:B:1262:THR:OG1	2.33	0.61
1:C:1272:GLN:HB3	1:C:1277:ARG:HB2	1.82	0.61
1:B:1351:LEU:HA	1:B:1354:LYS:NZ	2.15	0.61
1:A:1351:LEU:HA	1:A:1354:LYS:HE3	1.82	0.61
1:D:1450:ALA:HB1	1:D:1457:TRP:CD2	2.35	0.61
1:D:31:ILE:HD11	1:D:1018:ILE:HD11	1.80	0.61
1:D:833:ARG:HA	1:D:837:ILE:HB	1.83	0.61
1:A:1041:ILE:HG12	1:A:1126:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1450:ALA:HB1	1:C:1457:TRP:CD2	2.35	0.61
1:D:400:HIS:CD2	1:D:843:ALA:HB2	2.35	0.61
1:C:1351:LEU:HA	1:C:1354:LYS:HE3	1.83	0.61
1:A:1357:HIS:CE1	1:A:1409:ILE:HG21	2.36	0.61
1:B:1419:CYS:SG	1:B:1422:TRP:HE3	2.24	0.61
1:D:231:GLY:HA2	1:D:367:PRO:HG3	1.82	0.61
1:D:239:LYS:HD2	1:D:991:LEU:HD22	1.82	0.61
1:D:1234:PHE:HD1	1:D:1260:MET:SD	2.23	0.61
1:B:1059:LEU:HG	1:B:1094:LEU:HA	1.83	0.61
1:A:345:PHE:CD2	1:A:893:TRP:NE1	2.69	0.60
1:B:397:LEU:HD11	1:B:840:VAL:HG13	1.83	0.60
1:B:1247:ILE:HD12	1:B:1248:PRO:HD3	1.82	0.60
1:C:706:VAL:HB	1:C:803:PHE:HB2	1.83	0.60
1:A:1329:MET:HG2	1:A:1358:ILE:HD11	1.82	0.60
1:B:1068:HIS:NE2	1:B:1071:ASP:OD2	2.34	0.60
1:B:1337:GLU:HA	1:B:1340:ARG:HG3	1.84	0.60
1:B:1340:ARG:NE	1:B:1422:TRP:HD1	1.96	0.60
1:D:706:VAL:HB	1:D:803:PHE:HB2	1.82	0.60
1:D:1351:LEU:HA	1:D:1354:LYS:HE3	1.83	0.60
1:A:353:LEU:HD23	1:A:360:LEU:HD22	1.83	0.60
1:A:833:ARG:HA	1:A:837:ILE:HB	1.83	0.60
1:A:1214:MET:HA	1:A:1217:ILE:HD12	1.84	0.60
1:B:1328:PRO:HA	1:B:1357:HIS:HA	1.82	0.60
1:C:1059:LEU:HG	1:C:1094:LEU:HA	1.83	0.60
1:D:279:ILE:HD13	1:D:320:LYS:HE3	1.83	0.60
1:D:35:LEU:HD23	1:D:229:VAL:HG23	1.84	0.60
1:D:290:LEU:HD23	1:D:293:LEU:HD13	1.82	0.60
1:D:718:VAL:HG13	1:D:735:ILE:HD13	1.82	0.60
1:D:1059:LEU:HG	1:D:1094:LEU:HA	1.82	0.60
1:B:1214:MET:HA	1:B:1217:ILE:HD12	1.83	0.60
1:D:1357:HIS:CE1	1:D:1409:ILE:HG21	2.37	0.60
1:B:1090:TYR:HB2	1:B:1124:VAL:HG23	1.84	0.59
1:B:1402:HIS:NE2	1:D:767:LEU:CD1	2.65	0.59
1:C:387:LEU:HD21	1:C:861:LYS:CB	2.30	0.59
1:A:1077:ASN:ND2	1:C:818:ASP:OD2	2.35	0.59
1:B:239:LYS:HD2	1:B:991:LEU:HD22	1.84	0.59
1:C:49:LEU:HD21	1:C:64:LEU:HD13	1.84	0.59
1:C:858:SER:HA	1:C:861:LYS:CE	2.30	0.59
1:C:1044:HIS:O	1:C:1136:PRO:HD2	2.02	0.59
1:C:692:SER:HA	1:C:693:LYS:HZ2	1.68	0.59
1:A:1234:PHE:HD1	1:A:1260:MET:SD	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TYR:HE2	1:B:215:ARG:NH1	2.00	0.59
1:C:971:ASP:HB3	1:C:975:LYS:O	2.03	0.59
1:D:1061:LEU:O	1:D:1069:PHE:HB3	2.02	0.59
1:A:296:LYS:CE	1:A:331:SER:HA	2.33	0.59
1:B:1270:ARG:HH22	1:D:821:LYS:NZ	2.00	0.59
1:A:308:PHE:CE2	1:A:931:LYS:HA	2.38	0.59
1:C:1306:ILE:HD11	1:C:1457:TRP:CD1	2.36	0.59
1:C:1357:HIS:CE1	1:C:1409:ILE:HG21	2.37	0.59
1:B:706:VAL:HB	1:B:803:PHE:HB2	1.83	0.59
1:C:105:LEU:HD11	1:C:936:LEU:HD21	1.83	0.59
1:D:316:GLN:HB3	1:D:960:TYR:O	2.01	0.59
1:B:1216:ASN:HA	1:B:1219:MET:SD	2.43	0.59
1:B:1342:TRP:HB3	1:B:1356:TYR:CD1	2.38	0.59
1:A:407:LYS:HD3	1:A:885:VAL:HG22	1.85	0.58
1:B:99:ALA:HA	1:B:378:ARG:HD3	1.84	0.58
1:B:1388:ASP:OD2	1:B:1390:ASN:ND2	2.36	0.58
1:B:1268:TRP:CH2	1:B:1379:ARG:NH2	2.71	0.58
1:D:1306:ILE:HD11	1:D:1457:TRP:CD1	2.37	0.58
1:A:243:TYR:HB3	1:A:285:LEU:CG	2.25	0.58
1:B:340:GLY:HA2	1:B:343:GLU:HB2	1.84	0.58
1:B:1351:LEU:HB3	1:B:1354:LYS:HB2	1.84	0.58
1:C:397:LEU:HD11	1:C:840:VAL:HG13	1.84	0.58
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	2.19	0.58
1:C:840:VAL:HG12	1:C:844:LEU:HD22	1.85	0.58
1:C:1068:HIS:NE2	1:C:1071:ASP:OD2	2.36	0.58
1:C:1107:SER:CB	1:C:1120:ASP:HA	2.23	0.58
1:C:1214:MET:HA	1:C:1217:ILE:HD12	1.85	0.58
1:D:998:VAL:HG13	1:D:1002:TRP:HB2	1.85	0.58
1:D:1214:MET:HA	1:D:1217:ILE:HD12	1.85	0.58
1:D:1225:HIS:ND1	1:D:1308:ARG:HA	2.18	0.58
1:B:31:ILE:HD11	1:B:1018:ILE:HD11	1.85	0.58
1:C:64:LEU:HD12	1:C:67:ILE:HD11	1.85	0.58
1:D:42:PRO:CB	1:D:116:VAL:HG11	2.20	0.58
1:A:1380:GLN:HG3	1:C:712:ILE:HG21	1.85	0.58
1:D:340:GLY:HA2	1:D:343:GLU:HB2	1.85	0.58
1:D:1219:MET:HE1	1:D:1247:ILE:HG22	1.86	0.58
1:A:706:VAL:HB	1:A:803:PHE:HB2	1.84	0.58
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.36	0.58
1:C:239:LYS:HD2	1:C:991:LEU:HD22	1.86	0.58
1:C:963:VAL:HG22	1:C:981:ALA:HB2	1.85	0.58
1:A:231:GLY:HA2	1:A:367:PRO:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1331:ASP:HB3	1:D:1343:LYS:NZ	2.19	0.58
1:D:853:VAL:HG12	1:D:859:ALA:HA	1.86	0.57
1:B:1205:VAL:HB	1:B:1235:ILE:HG12	1.86	0.57
1:A:1272:GLN:HB3	1:A:1277:ARG:HB2	1.84	0.57
1:B:353:LEU:HG	1:B:914:ALA:HA	1.85	0.57
1:D:1068:HIS:NE2	1:D:1071:ASP:OD2	2.37	0.57
1:D:110:ARG:NH1	1:D:976:VAL:HG21	2.20	0.57
1:B:1198:ALA:HB3	1:B:1231:LYS:HB2	1.86	0.57
1:C:122:TYR:OH	1:C:215:ARG:NH1	2.38	0.57
1:B:1075:MET:HB3	1:B:1379:ARG:NH2	2.20	0.57
1:C:238:LEU:HD21	1:C:959:PHE:HE2	1.69	0.57
1:C:1331:ASP:HB3	1:C:1343:LYS:NZ	2.19	0.57
1:A:1082:GLN:HG2	1:A:1263:TYR:CZ	2.39	0.57
1:B:718:VAL:HG13	1:B:735:ILE:HD13	1.86	0.57
1:A:718:VAL:HG13	1:A:735:ILE:HD13	1.86	0.57
1:B:1270:ARG:NH2	1:D:821:LYS:NZ	2.53	0.56
1:A:346:LEU:HG	1:A:893:TRP:CZ2	2.39	0.56
1:D:1134:LEU:C	1:D:1136:PRO:HD3	2.30	0.56
1:A:1021:ILE:HG23	1:A:1025:ARG:HG3	1.86	0.56
1:B:666:GLU:OE1	1:D:664:LYS:O	2.23	0.56
1:B:821:LYS:HZ1	1:D:1270:ARG:HH12	1.54	0.56
1:B:930:LEU:HD23	1:B:933:LEU:HD12	1.86	0.56
1:D:119:HIS:CE1	1:D:172:PHE:HB2	2.40	0.56
1:C:718:VAL:HG13	1:C:735:ILE:HD13	1.85	0.56
1:C:1275:LYS:O	1:C:1279:ILE:HG13	2.05	0.56
1:B:237:VAL:HA	1:B:958:ARG:HA	1.88	0.56
1:C:340:GLY:HA2	1:C:343:GLU:HB2	1.87	0.56
1:D:387:LEU:CD2	1:D:861:LYS:HB2	2.30	0.56
1:D:64:LEU:HD12	1:D:67:ILE:HD11	1.87	0.56
1:D:1288:ASP:HB3	1:D:1369:PHE:HD2	1.69	0.56
1:B:64:LEU:HD12	1:B:67:ILE:HD11	1.87	0.56
1:C:78:ASP:HB2	1:C:975:LYS:HA	1.87	0.56
1:C:1197:HIS:CE1	1:C:1231:LYS:NZ	2.74	0.56
1:C:1225:HIS:ND1	1:C:1308:ARG:HA	2.20	0.56
1:D:993:VAL:HG13	1:D:1014:ASP:HA	1.87	0.56
1:B:1287:LEU:HD22	1:B:1364:VAL:HG11	1.88	0.56
1:A:64:LEU:HD12	1:A:67:ILE:HD11	1.86	0.56
1:A:1214:MET:CE	1:A:1457:TRP:HE1	2.16	0.56
1:B:1280:TRP:HA	1:B:1283:LYS:HD3	1.87	0.56
1:B:1404:GLN:CG	1:B:1409:ILE:HB	2.30	0.56
2:E:1:NAG:H61	2:E:2:NAG:C7	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ILE:HG13	1:A:364:GLN:HB2	1.87	0.56
1:A:1013:LEU:HD21	1:A:1241:PRO:HD3	1.86	0.56
1:B:703:LEU:HB2	1:B:806:LEU:HD12	1.88	0.56
1:B:46:VAL:HG13	1:B:116:VAL:HG21	1.88	0.55
1:B:1253:GLU:HG3	1:B:1467:LEU:HD11	1.86	0.55
1:D:975:LYS:HG3	1:D:976:VAL:H	1.70	0.55
1:B:1270:ARG:HH22	1:D:821:LYS:HZ2	1.54	0.55
1:C:378:ARG:HD2	1:C:909:THR:HG21	1.88	0.55
1:D:1207:SER:HB2	1:D:1279:ILE:HD11	1.89	0.55
1:C:105:LEU:CG	1:C:966:SER:HA	2.34	0.55
1:C:853:VAL:HG12	1:C:859:ALA:HA	1.88	0.55
1:C:1374:ALA:HA	1:C:1377:ARG:HE	1.71	0.55
1:A:338:HIS:CE1	1:A:897:TYR:H	2.24	0.55
1:A:1309:THR:HG21	1:A:1432:ARG:HD3	1.87	0.55
1:D:1236:GLU:HG2	1:D:1244:LYS:NZ	2.22	0.55
1:B:1270:ARG:NH2	1:D:821:LYS:HZ1	2.04	0.55
1:A:380:LEU:HD21	1:A:869:SER:CB	2.37	0.55
1:C:397:LEU:HD13	1:C:844:LEU:HD13	1.88	0.55
1:C:1040:LEU:HD22	1:C:1082:GLN:HB2	1.89	0.55
1:D:703:LEU:HB2	1:D:806:LEU:HD12	1.89	0.55
1:A:308:PHE:HE2	1:A:931:LYS:HA	1.72	0.55
1:B:1302:ASP:HB3	1:B:1360:ALA:HB1	1.88	0.55
1:C:1134:LEU:O	1:C:1136:PRO:HD3	2.07	0.55
1:D:1225:HIS:CE1	1:D:1308:ARG:HA	2.42	0.55
1:C:703:LEU:HB2	1:C:806:LEU:HD12	1.88	0.55
1:C:1224:HIS:HE1	1:C:1463:GLU:OE1	1.90	0.55
1:D:52:ALA:HB1	1:D:89:LEU:HD21	1.89	0.55
1:A:1094:LEU:HD11	1:A:1105:LEU:H	1.71	0.55
1:D:1197:HIS:CE1	1:D:1231:LYS:NZ	2.74	0.55
1:C:1374:ALA:HA	1:C:1377:ARG:HG3	1.89	0.55
1:D:296:LYS:HZ3	1:D:326:GLY:CA	2.19	0.55
1:A:1219:MET:HE1	1:A:1247:ILE:HG22	1.89	0.54
1:A:1107:SER:CB	1:A:1120:ASP:HA	2.26	0.54
1:B:882:ALA:H	1:B:883:PRO:CD	2.20	0.54
1:D:930:LEU:HD23	1:D:933:LEU:HD12	1.90	0.54
1:B:765:ARG:HD2	1:D:1391:SER:HB3	1.88	0.54
1:B:1357:HIS:CE1	1:B:1404:GLN:NE2	2.76	0.54
1:B:1454:VAL:HG13	1:B:1456:GLU:HG2	1.88	0.54
1:A:312:LEU:O	1:A:316:GLN:HG2	2.07	0.54
1:B:1094:LEU:HD11	1:B:1105:LEU:H	1.72	0.54
1:A:703:LEU:HB2	1:A:806:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:GLU:O	1:B:667:LEU:HB2	2.07	0.54
1:B:1205:VAL:HB	1:B:1235:ILE:CG1	2.37	0.54
1:C:1450:ALA:HB1	1:C:1457:TRP:CG	2.42	0.54
1:B:837:ILE:HG12	1:B:863:THR:HG21	1.88	0.54
1:C:279:ILE:HD13	1:C:320:LYS:HE3	1.88	0.54
1:D:78:ASP:HB2	1:D:975:LYS:CA	2.16	0.54
1:D:230:ASN:HD22	1:D:964:LEU:HG	1.72	0.54
1:D:376:ARG:HH22	1:D:874:LEU:N	2.05	0.54
1:D:1309:THR:HG21	1:D:1432:ARG:HD3	1.89	0.54
1:D:1450:ALA:HB1	1:D:1457:TRP:CG	2.43	0.54
1:B:279:ILE:HD13	1:B:320:LYS:HE3	1.90	0.54
1:D:999:PRO:O	1:D:1002:TRP:HB2	2.08	0.54
1:D:1094:LEU:HD11	1:D:1105:LEU:H	1.73	0.54
1:A:279:ILE:HD13	1:A:320:LYS:HE3	1.90	0.54
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.43	0.54
1:A:1450:ALA:HB1	1:A:1457:TRP:CG	2.42	0.54
1:B:669:VAL:HG22	1:B:809:ARG:HG3	1.90	0.54
1:A:339:ARG:HH12	1:A:946:ASN:HB2	1.73	0.54
1:B:1352:LYS:H	1:B:1354:LYS:NZ	2.06	0.53
1:C:1044:HIS:N	1:C:1044:HIS:CD2	2.75	0.53
1:D:715:GLN:HG3	1:D:766:PHE:HZ	1.73	0.53
1:B:1361:LEU:HD22	1:B:1417:LEU:HD13	1.90	0.53
1:C:1309:THR:HG21	1:C:1432:ARG:HD3	1.89	0.53
1:C:1331:ASP:CB	1:C:1343:LYS:HZ1	2.21	0.53
1:A:245:VAL:HB	1:A:287:LYS:HA	1.89	0.53
1:C:1374:ALA:HB2	1:C:1377:ARG:HH21	1.73	0.53
1:A:1368:ARG:O	1:A:1368:ARG:HD3	2.09	0.53
1:D:673:ASN:CA	1:D:861:LYS:HD2	2.33	0.53
1:B:988:ARG:HG2	1:B:1018:ILE:HG22	1.89	0.53
1:C:31:ILE:HD12	1:C:236:LEU:HD11	1.90	0.53
1:A:1007:LYS:O	1:A:1241:PRO:HB3	2.09	0.53
1:B:1299:ILE:HG23	1:B:1363:VAL:HG22	1.91	0.53
1:C:1225:HIS:CE1	1:C:1308:ARG:HA	2.43	0.53
1:C:1467:LEU:HD12	1:C:1470:ARG:HE	1.73	0.53
1:A:929:VAL:O	1:A:933:LEU:HG	2.08	0.53
1:B:1270:ARG:CZ	1:D:821:LYS:NZ	2.71	0.53
1:C:1286:PHE:HB3	1:C:1290:LEU:HD13	1.91	0.53
1:B:179:GLY:HA3	1:B:210:ALA:CA	2.39	0.53
1:B:686:VAL:HG11	1:B:736:VAL:HG22	1.91	0.53
1:C:354:TRP:CZ3	1:C:890:PHE:HB3	2.44	0.53
1:C:363:ARG:NH1	1:C:879:PHE:CE1	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:THR:HG21	1:D:884:THR:HG22	1.91	0.53
1:C:316:GLN:HB2	1:C:961:ARG:HD3	1.90	0.53
1:D:354:TRP:CZ3	1:D:890:PHE:HB3	2.44	0.53
1:D:1038:HIS:CD2	1:D:1085:ALA:HA	2.43	0.53
1:D:1331:ASP:CB	1:D:1343:LYS:HZ1	2.22	0.53
1:B:122:TYR:CE2	1:B:215:ARG:NH1	2.77	0.53
1:D:37:ALA:O	1:D:226:SER:OG	2.27	0.53
1:D:375:THR:O	1:D:378:ARG:HB3	2.09	0.53
1:A:308:PHE:CZ	1:A:931:LYS:HG3	2.44	0.52
1:A:1467:LEU:HD12	1:A:1470:ARG:HE	1.74	0.52
1:B:237:VAL:HG22	1:B:958:ARG:HB3	1.91	0.52
1:B:125:ALA:O	1:B:1064:GLU:HB2	2.08	0.52
1:C:1094:LEU:HD11	1:C:1105:LEU:H	1.73	0.52
1:B:1352:LYS:N	1:B:1354:LYS:HZ3	2.08	0.52
1:B:354:TRP:CZ3	1:B:890:PHE:HB3	2.45	0.52
1:D:763:PHE:HD1	1:D:768:ASP:HB3	1.74	0.52
1:A:109:LEU:HD21	1:A:964:LEU:CD1	2.40	0.52
1:A:179:GLY:HA3	1:A:210:ALA:CA	2.37	0.52
1:A:1197:HIS:CE1	1:A:1231:LYS:NZ	2.77	0.52
1:B:1003:LEU:HA	1:B:1264:LYS:HZ2	1.74	0.52
1:D:660:PHE:O	1:D:663:ASP:OD1	2.28	0.52
1:B:349:GLY:CA	1:B:948:THR:HB	2.37	0.52
1:B:879:PHE:N	1:B:879:PHE:CD1	2.75	0.52
1:B:1392:LEU:HD22	1:B:1398:ASP:HB3	1.91	0.52
1:C:874:LEU:HB3	1:C:879:PHE:HD2	1.74	0.52
1:D:669:VAL:HG22	1:D:809:ARG:HG3	1.91	0.52
1:A:60:TYR:CD1	1:A:174:ARG:NH1	2.78	0.52
1:B:60:TYR:CD1	1:B:174:ARG:NH1	2.78	0.52
1:B:965:SER:OG	1:B:967:SER:O	2.24	0.52
1:D:115:ARG:NH2	1:D:174:ARG:NH2	2.45	0.52
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.75	0.52
1:A:1094:LEU:HG	1:A:1105:LEU:HD23	1.91	0.52
1:C:1214:MET:CE	1:C:1457:TRP:HE1	2.18	0.52
1:C:930:LEU:HD23	1:C:933:LEU:HD12	1.92	0.52
1:C:992:LEU:O	1:C:1014:ASP:O	2.28	0.52
1:A:244:ILE:HD11	1:A:954:LEU:HB2	1.92	0.52
1:B:296:LYS:HZ3	1:B:326:GLY:HA2	1.74	0.52
1:B:384:VAL:HG12	1:B:389:LEU:HB2	1.91	0.52
1:C:1016:LEU:HD11	1:C:1030:VAL:HG11	1.91	0.52
1:D:1467:LEU:HD12	1:D:1470:ARG:HE	1.75	0.52
1:A:338:HIS:CE1	1:A:894:ASN:O	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:HG12	1:C:183:VAL:HG12	1.92	0.51
1:A:296:LYS:CD	1:A:331:SER:HA	2.40	0.51
1:D:381:ILE:HG21	1:D:909:THR:HA	1.92	0.51
1:B:1234:PHE:HB2	1:B:1260:MET:HG2	1.92	0.51
1:D:45:LEU:HA	1:D:81:LEU:HD21	1.91	0.51
1:D:60:TYR:CD1	1:D:174:ARG:NH1	2.79	0.51
1:D:334:PHE:HB3	1:D:897:TYR:CZ	2.46	0.51
1:D:700:TRP:HB3	1:D:856:PRO:HA	1.92	0.51
1:A:48:LEU:HD21	1:A:82:TYR:HA	1.91	0.51
1:B:1219:MET:O	1:B:1223:MET:HG2	2.11	0.51
1:C:1219:MET:HE1	1:C:1247:ILE:HG22	1.91	0.51
1:B:400:HIS:CD2	1:B:843:ALA:CB	2.94	0.51
1:B:1418:TRP:NE1	1:B:1427:THR:OG1	2.29	0.51
1:C:963:VAL:CG1	1:C:979:LEU:HB3	2.41	0.51
1:D:1040:LEU:HD22	1:D:1082:GLN:HB2	1.92	0.51
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.92	0.51
1:B:879:PHE:HB2	1:B:880:ASP:CA	2.37	0.51
1:B:995:GLY:O	1:B:996:MET:HG3	2.10	0.51
1:B:1235:ILE:HB	1:B:1238:PHE:HE2	1.75	0.51
1:C:119:HIS:ND1	1:C:216:TYR:CD2	2.78	0.51
1:C:1416:TRP:CZ2	1:C:1432:ARG:NH1	2.79	0.51
1:D:1288:ASP:HB3	1:D:1369:PHE:CD2	2.45	0.51
1:A:1416:TRP:CZ2	1:A:1432:ARG:NH1	2.79	0.51
1:B:144:ILE:HG12	1:B:183:VAL:HG12	1.93	0.51
1:C:392:GLN:HE22	1:C:891:LYS:NZ	2.09	0.51
1:C:763:PHE:HD1	1:C:768:ASP:HB3	1.75	0.51
1:C:998:VAL:HG21	1:C:1004:VAL:HG21	1.93	0.51
1:D:958:ARG:NH1	1:D:960:TYR:CE1	2.79	0.51
1:C:686:VAL:HG11	1:C:736:VAL:HG22	1.93	0.51
1:D:392:GLN:HE22	1:D:891:LYS:HZ1	1.58	0.51
1:B:381:ILE:HG21	1:B:909:THR:HA	1.93	0.51
1:B:1213:ARG:NH2	1:B:1451:ARG:HH12	2.09	0.51
1:B:1302:ASP:O	1:B:1302:ASP:CG	2.54	0.51
1:C:313:LYS:O	1:C:316:GLN:HG2	2.11	0.51
1:C:715:GLN:HG3	1:C:766:PHE:HZ	1.74	0.51
1:B:296:LYS:HE2	1:B:331:SER:CA	2.41	0.51
1:B:1199:GLU:OE2	1:B:1228:HIS:ND1	2.37	0.50
1:C:737:HIS:NE2	1:C:749:LEU:HD12	2.25	0.50
1:D:400:HIS:HD2	1:D:402:GLU:HB2	1.76	0.50
2:E:1:NAG:C6	2:E:2:NAG:HN2	2.23	0.50
1:A:1090:TYR:HB2	1:A:1124:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:932:VAL:HG11	1:B:964:LEU:HG	1.92	0.50
1:B:1296:ASP:O	1:B:1366:LEU:HB2	2.11	0.50
1:C:119:HIS:ND1	1:C:216:TYR:HD2	2.09	0.50
1:C:296:LYS:HE2	1:C:331:SER:CA	2.41	0.50
1:A:1331:ASP:HB3	1:A:1343:LYS:NZ	2.26	0.50
1:B:244:ILE:HD11	1:B:954:LEU:HB2	1.93	0.50
1:B:1108:VAL:HG12	1:B:1134:LEU:HD22	1.93	0.50
1:B:1265:TRP:NE1	1:B:1269:LEU:HD23	2.26	0.50
1:B:1319:LEU:HG	1:B:1320:ASP:N	2.26	0.50
1:C:60:TYR:CD1	1:C:174:ARG:NH1	2.79	0.50
1:D:881:ASN:O	1:D:881:ASN:OD1	2.28	0.50
1:D:963:VAL:CG2	1:D:981:ALA:HB2	2.42	0.50
1:C:1342:TRP:HE1	1:C:1343:LYS:HE3	1.77	0.50
1:D:682:LEU:HD22	1:D:788:LEU:HA	1.92	0.50
1:B:143:LEU:HD13	1:B:161:VAL:HG21	1.94	0.50
1:B:1094:LEU:HG	1:B:1105:LEU:HD23	1.93	0.50
1:C:700:TRP:HB3	1:C:856:PRO:HA	1.93	0.50
1:D:316:GLN:NE2	1:D:961:ARG:HH11	2.09	0.50
1:D:1224:HIS:HE1	1:D:1463:GLU:OE1	1.95	0.50
1:D:1416:TRP:CZ2	1:D:1432:ARG:NH1	2.79	0.50
1:B:42:PRO:HB3	1:B:116:VAL:HG11	1.94	0.50
1:C:381:ILE:HG21	1:C:909:THR:HA	1.94	0.50
1:D:111:THR:O	1:D:114:PRO:HD2	2.12	0.50
1:D:1134:LEU:O	1:D:1136:PRO:HD3	2.11	0.50
1:B:700:TRP:HB3	1:B:856:PRO:HA	1.94	0.50
1:C:75:ALA:HB1	1:C:81:LEU:HG	1.94	0.50
1:C:334:PHE:HB3	1:C:897:TYR:CZ	2.47	0.50
1:D:1199:GLU:OE2	1:D:1228:HIS:ND1	2.44	0.50
1:A:1098:ARG:NE	1:A:1152:PRO:HD3	2.19	0.50
1:B:78:ASP:CB	1:B:975:LYS:HA	2.36	0.50
1:B:312:LEU:O	1:B:316:GLN:HB3	2.11	0.50
1:B:715:GLN:HG3	1:B:766:PHE:HZ	1.76	0.50
1:B:1352:LYS:NZ	1:D:774:GLU:HB3	2.27	0.50
1:C:1058:GLN:HB3	1:C:1293:LEU:CD1	2.42	0.50
1:B:56:ASN:OD1	1:B:58:THR:OG1	2.30	0.50
1:B:334:PHE:HB3	1:B:897:TYR:CZ	2.47	0.50
1:A:686:VAL:HG11	1:A:736:VAL:HG22	1.93	0.49
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.94	0.49
1:B:1319:LEU:HG	1:B:1320:ASP:H	1.77	0.49
1:C:400:HIS:CD2	1:C:843:ALA:CB	2.95	0.49
1:D:179:GLY:HA3	1:D:210:ALA:CA	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:GLN:NE2	1:D:961:ARG:NH1	2.60	0.49
1:A:1005:THR:HG22	1:A:1237:GLN:HB3	1.94	0.49
1:A:1224:HIS:HE1	1:A:1463:GLU:OE1	1.95	0.49
1:B:1087:PRO:HA	1:B:1126:LEU:HG	1.94	0.49
1:B:1270:ARG:NH1	1:D:821:LYS:HZ3	1.99	0.49
1:B:1295:LEU:HD11	1:B:1298:VAL:HB	1.93	0.49
1:C:244:ILE:HD11	1:C:954:LEU:HB2	1.93	0.49
1:D:1351:LEU:HA	1:D:1354:LYS:CE	2.42	0.49
1:A:1351:LEU:HA	1:A:1354:LYS:CE	2.42	0.49
1:B:45:LEU:HA	1:B:48:LEU:HD12	1.94	0.49
1:B:115:ARG:HA	1:B:1127:MET:HB2	1.94	0.49
1:D:110:ARG:O	1:D:113:THR:OG1	2.27	0.49
1:D:737:HIS:NE2	1:D:749:LEU:HD12	2.27	0.49
1:A:715:GLN:HG3	1:A:766:PHE:HZ	1.77	0.49
1:A:1105:LEU:CA	1:A:1138:LEU:HG	2.30	0.49
1:B:763:PHE:HD1	1:B:768:ASP:HB3	1.76	0.49
1:B:1323:PRO:CB	1:B:1369:PHE:HA	2.41	0.49
1:C:143:LEU:HD13	1:C:161:VAL:HG21	1.95	0.49
1:C:1467:LEU:HD12	1:C:1470:ARG:NE	2.27	0.49
1:D:686:VAL:HG11	1:D:736:VAL:HG22	1.94	0.49
1:D:1081:PHE:HE2	1:D:1134:LEU:HD12	1.76	0.49
1:A:1450:ALA:HB1	1:A:1457:TRP:CE2	2.47	0.49
1:C:179:GLY:HA3	1:C:210:ALA:CA	2.39	0.49
1:D:44:TYR:CE2	1:D:110:ARG:NH2	2.77	0.49
1:C:349:GLY:CA	1:C:948:THR:HB	2.38	0.49
1:C:1199:GLU:OE2	1:C:1228:HIS:ND1	2.46	0.49
1:D:109:LEU:HD21	1:D:964:LEU:HD21	1.93	0.49
1:D:1342:TRP:HE1	1:D:1343:LYS:HE3	1.77	0.49
1:A:384:VAL:HG22	1:A:865:VAL:HG11	1.95	0.49
1:D:120:TYR:CE1	1:D:218:ARG:HA	2.48	0.49
1:D:1214:MET:CE	1:D:1457:TRP:HE1	2.18	0.49
1:B:1098:ARG:HE	1:B:1152:PRO:HB3	1.77	0.49
1:C:89:LEU:HD22	1:C:95:MET:HG3	1.94	0.49
1:A:339:ARG:HH22	1:A:946:ASN:HB2	1.78	0.49
1:A:669:VAL:HG22	1:A:809:ARG:HG3	1.94	0.48
1:B:1352:LYS:N	1:B:1354:LYS:NZ	2.61	0.48
1:B:1375:GLY:O	1:B:1379:ARG:HD2	2.13	0.48
1:C:392:GLN:HE22	1:C:891:LYS:HZ1	1.58	0.48
1:A:339:ARG:NH1	1:A:946:ASN:HB2	2.27	0.48
1:A:380:LEU:HD21	1:A:869:SER:HB3	1.95	0.48
1:C:407:LYS:HE3	1:C:870:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:LEU:HD22	1:C:788:LEU:HA	1.95	0.48
1:D:349:GLY:HA2	1:D:917:ASN:HB2	1.94	0.48
1:A:315:THR:HG23	1:A:316:GLN:HE21	1.77	0.48
1:A:358:LEU:HD22	1:A:884:THR:HB	1.95	0.48
1:A:1011:ASP:OD2	1:A:1021:ILE:HG12	2.13	0.48
1:A:1199:GLU:OE2	1:A:1228:HIS:ND1	2.45	0.48
1:B:737:HIS:NE2	1:B:749:LEU:HD12	2.27	0.48
1:B:1040:LEU:HD22	1:B:1082:GLN:HB2	1.94	0.48
1:A:1376:ASP:O	1:A:1380:GLN:HG2	2.12	0.48
1:B:29:PRO:HB2	1:B:986:VAL:O	2.14	0.48
1:B:78:ASP:HA	1:B:81:LEU:HD23	1.94	0.48
1:B:1075:MET:HE2	1:B:1289:VAL:HG11	1.95	0.48
1:C:349:GLY:HA2	1:C:917:ASN:HB2	1.96	0.48
1:D:392:GLN:HE22	1:D:891:LYS:NZ	2.10	0.48
1:D:1094:LEU:HG	1:D:1105:LEU:HD23	1.94	0.48
1:A:368:PHE:O	1:A:372:ASP:OD1	2.32	0.48
1:B:682:LEU:HD22	1:B:788:LEU:HA	1.94	0.48
1:B:1357:HIS:H	1:B:1401:ASN:HD21	1.60	0.48
1:B:1459:LYS:HZ3	1:B:1460:TYR:HE1	1.62	0.48
1:D:1377:ARG:HA	1:D:1380:GLN:CG	2.44	0.48
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.95	0.48
1:A:334:PHE:O	1:A:337:GLU:HG2	2.12	0.48
1:B:1376:ASP:CA	1:B:1379:ARG:HD3	2.18	0.48
1:C:353:LEU:HG	1:C:914:ALA:HA	1.95	0.48
1:C:363:ARG:NH1	1:C:879:PHE:CZ	2.82	0.48
1:D:1087:PRO:HA	1:D:1126:LEU:HG	1.95	0.48
1:D:1377:ARG:HA	1:D:1380:GLN:HG2	1.94	0.48
1:D:1450:ALA:HB1	1:D:1457:TRP:CE2	2.49	0.48
1:A:700:TRP:HB3	1:A:856:PRO:HA	1.96	0.48
1:B:372:ASP:O	1:B:376:ARG:HG3	2.13	0.48
1:D:56:ASN:OD1	1:D:58:THR:OG1	2.32	0.48
1:A:334:PHE:HB3	1:A:897:TYR:CZ	2.48	0.48
1:D:1357:HIS:CE1	1:D:1409:ILE:CG2	2.97	0.48
1:A:110:ARG:CZ	1:A:227:LEU:HD11	2.44	0.48
1:A:371:VAL:HA	1:A:374:LEU:HD23	1.96	0.48
1:A:1357:HIS:CE1	1:A:1409:ILE:CG2	2.97	0.48
1:B:184:ILE:HG12	1:B:213:ARG:HG3	1.96	0.48
1:C:1206:ALA:HB1	1:C:1211:TYR:HB3	1.96	0.48
1:C:1276:GLN:HA	1:C:1279:ILE:HD12	1.94	0.48
1:C:1357:HIS:CE1	1:C:1409:ILE:CG2	2.97	0.48
1:D:244:ILE:HD11	1:D:954:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:PHE:HB3	1:C:893:TRP:HE1	1.79	0.48
1:A:874:LEU:H	1:A:875:PRO:CA	2.13	0.47
1:B:664:LYS:HB3	1:D:666:GLU:OE2	2.14	0.47
1:A:143:LEU:HD13	1:A:161:VAL:HG21	1.96	0.47
1:B:392:GLN:HE22	1:B:891:LYS:HZ1	1.62	0.47
1:C:669:VAL:HG22	1:C:809:ARG:HG3	1.95	0.47
1:A:737:HIS:NE2	1:A:749:LEU:HD12	2.28	0.47
1:A:795:SER:HB3	1:A:797:MET:HE3	1.96	0.47
1:A:1402:HIS:HE1	1:C:770:GLU:OE1	1.97	0.47
1:D:296:LYS:HE2	1:D:331:SER:CA	2.42	0.47
1:D:1467:LEU:HD12	1:D:1470:ARG:NE	2.29	0.47
1:A:56:ASN:OD1	1:A:58:THR:OG1	2.33	0.47
1:B:230:ASN:HD22	1:B:964:LEU:HA	1.78	0.47
1:C:988:ARG:HB3	1:C:1019:LYS:HB2	1.95	0.47
1:C:1450:ALA:HB1	1:C:1457:TRP:CE2	2.49	0.47
1:A:184:ILE:HG12	1:A:213:ARG:HG3	1.96	0.47
1:B:387:LEU:HD22	1:B:862:LEU:HG	1.96	0.47
1:B:392:GLN:HE22	1:B:891:LYS:NZ	2.11	0.47
1:B:1301:VAL:HG13	1:B:1305:GLN:HB2	1.95	0.47
1:B:1335:GLU:HG2	1:B:1336:MET:SD	2.55	0.47
1:C:311:LEU:HG	1:C:927:VAL:HG11	1.97	0.47
1:C:1134:LEU:C	1:C:1136:PRO:HD3	2.39	0.47
1:A:52:ALA:HB1	1:A:89:LEU:HD21	1.97	0.47
1:A:296:LYS:HE2	1:A:331:SER:CA	2.41	0.47
1:A:951:ILE:HG22	1:A:953:GLU:O	2.15	0.47
1:B:1357:HIS:NE2	1:B:1411:THR:CG2	2.68	0.47
1:C:184:ILE:HG12	1:C:213:ARG:HG3	1.96	0.47
1:C:924:GLN:HE22	1:C:956:VAL:HG11	1.79	0.47
1:C:963:VAL:HG12	1:C:979:LEU:HB3	1.97	0.47
1:C:1108:VAL:HG23	1:C:1122:THR:HA	1.97	0.47
1:C:1336:MET:SD	1:C:1421:THR:O	2.73	0.47
1:D:143:LEU:HD13	1:D:161:VAL:HG21	1.96	0.47
1:D:144:ILE:HG12	1:D:183:VAL:HG12	1.95	0.47
1:D:349:GLY:CA	1:D:948:THR:HB	2.38	0.47
1:D:988:ARG:HG2	1:D:1018:ILE:HG22	1.96	0.47
1:D:1080:TYR:OH	1:D:1082:GLN:NE2	2.29	0.47
1:D:1206:ALA:HB1	1:D:1211:TYR:HB3	1.97	0.47
1:D:1336:MET:SD	1:D:1421:THR:O	2.73	0.47
1:A:682:LEU:HD22	1:A:788:LEU:HA	1.95	0.47
1:C:1094:LEU:HG	1:C:1105:LEU:HD23	1.95	0.47
1:D:29:PRO:HB2	1:D:986:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLU:O	1:A:663:ASP:CG	2.58	0.47
1:B:43:PRO:O	1:B:46:VAL:HG12	2.15	0.47
1:B:297:ALA:HB1	1:B:314:LEU:HD21	1.97	0.47
1:B:907:THR:O	1:B:938:GLY:HA2	2.15	0.47
1:D:878:ILE:O	1:D:882:ALA:O	2.32	0.47
1:A:1296:ASP:O	1:A:1366:LEU:HB2	2.14	0.47
1:B:917:ASN:OD1	1:B:947:PRO:HA	2.15	0.47
1:B:1466:GLU:HA	1:B:1469:ARG:CD	2.32	0.47
1:D:298:ALA:HB2	1:D:918:PRO:HG2	1.96	0.47
1:A:1467:LEU:HD12	1:A:1470:ARG:NE	2.29	0.46
1:B:109:LEU:HB3	1:B:368:PHE:CE1	2.50	0.46
1:B:348:GLU:HB2	1:B:947:PRO:O	2.15	0.46
1:D:184:ILE:HG12	1:D:213:ARG:HG3	1.97	0.46
1:A:345:PHE:CD1	1:A:345:PHE:C	2.92	0.46
1:B:345:PHE:HB3	1:B:893:TRP:HE1	1.81	0.46
1:B:349:GLY:HA2	1:B:917:ASN:HB2	1.98	0.46
1:B:1090:TYR:HB2	1:B:1124:VAL:O	2.15	0.46
1:B:1108:VAL:HG23	1:B:1122:THR:HA	1.96	0.46
1:B:1357:HIS:HE1	1:B:1404:GLN:HE22	1.63	0.46
1:C:135:GLN:HE22	1:C:148:GLN:HE21	1.63	0.46
1:D:917:ASN:OD1	1:D:947:PRO:HA	2.15	0.46
1:B:1105:LEU:CA	1:B:1138:LEU:HG	2.30	0.46
1:B:1280:TRP:CD1	1:B:1283:LYS:NZ	2.82	0.46
1:D:384:VAL:HG12	1:D:389:LEU:HB2	1.97	0.46
1:A:109:LEU:HD21	1:A:964:LEU:HD13	1.97	0.46
1:B:687:PRO:HD2	1:B:735:ILE:O	2.15	0.46
1:C:281:ASP:OD1	1:C:988:ARG:NH1	2.44	0.46
1:C:795:SER:HB3	1:C:797:MET:HE3	1.98	0.46
1:D:110:ARG:HH12	1:D:976:VAL:HG21	1.80	0.46
1:A:286:GLU:HB2	1:A:289:GLU:OE2	2.16	0.46
1:B:1391:SER:HB3	1:D:765:ARG:HD2	1.97	0.46
1:B:1420:GLU:N	1:B:1437:CYS:SG	2.89	0.46
1:C:672:VAL:HB	1:C:861:LYS:HA	1.97	0.46
1:C:1319:LEU:HD12	1:C:1365:ASP:HB2	1.98	0.46
1:C:384:VAL:HG12	1:C:389:LEU:HB2	1.98	0.46
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.98	0.46
1:B:398:LEU:HB3	1:B:886:ARG:HD3	1.98	0.46
1:B:1324:TYR:HA	1:B:1364:VAL:HA	1.98	0.46
1:C:693:LYS:HZ3	1:C:693:LYS:N	2.08	0.46
1:C:1295:LEU:HD21	1:C:1298:VAL:HG22	1.97	0.46
1:D:1236:GLU:CG	1:D:1244:LYS:NZ	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1276:GLN:HA	1:D:1279:ILE:HD12	1.98	0.46
1:A:335:GLU:HA	1:A:338:HIS:HB2	1.97	0.46
1:D:110:ARG:CZ	1:D:227:LEU:HD11	2.45	0.46
1:D:345:PHE:HB3	1:D:893:TRP:HE1	1.81	0.46
1:D:400:HIS:CD2	1:D:843:ALA:CB	2.99	0.46
1:A:1342:TRP:HE1	1:A:1343:LYS:HE3	1.80	0.46
1:B:1351:LEU:HD22	1:B:1354:LYS:HE2	1.97	0.46
1:C:115:ARG:HA	1:C:1127:MET:HB2	1.98	0.46
1:C:1092:ILE:O	1:C:1122:THR:OG1	2.34	0.46
1:C:1314:LEU:HD11	1:C:1412:LEU:HD13	1.98	0.46
1:D:878:ILE:HA	1:D:879:PHE:HA	1.77	0.46
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.46	0.46
1:C:31:ILE:HG12	1:C:1030:VAL:HB	1.96	0.46
1:C:45:LEU:HD12	1:C:81:LEU:HD21	1.97	0.46
1:D:998:VAL:HG13	1:D:1002:TRP:CB	2.46	0.46
1:A:666:GLU:O	1:A:667:LEU:HB2	2.15	0.45
1:B:1465:ALA:C	1:B:1469:ARG:HE	2.23	0.45
1:C:348:GLU:HB2	1:C:947:PRO:O	2.16	0.45
1:C:1335:GLU:HG2	1:C:1336:MET:SD	2.56	0.45
1:B:1092:ILE:O	1:B:1122:THR:OG1	2.33	0.45
1:D:1115:PRO:HG3	1:D:1137:ARG:NE	2.31	0.45
1:B:338:HIS:CD2	1:B:341:ASN:ND2	2.79	0.45
1:C:1234:PHE:CD1	1:C:1260:MET:SD	3.08	0.45
1:C:1351:LEU:HA	1:C:1354:LYS:CE	2.44	0.45
1:D:297:ALA:HB1	1:D:314:LEU:HD21	1.98	0.45
1:D:375:THR:HA	1:D:378:ARG:HB2	1.98	0.45
1:A:75:ALA:HB1	1:A:81:LEU:CB	2.46	0.45
1:B:1319:LEU:H	1:B:1319:LEU:HD23	1.82	0.45
1:D:1108:VAL:HG23	1:D:1122:THR:HA	1.98	0.45
1:A:687:PRO:HD2	1:A:735:ILE:O	2.16	0.45
1:B:795:SER:HB3	1:B:797:MET:HE3	1.97	0.45
1:B:1295:LEU:HB3	1:B:1366:LEU:HG	1.98	0.45
1:C:1469:ARG:HA	1:C:1472:ARG:HB2	1.98	0.45
1:D:1469:ARG:HA	1:D:1472:ARG:HB2	1.97	0.45
1:A:311:LEU:O	1:A:315:THR:HG22	2.16	0.45
1:A:716:GLU:CD	1:C:1384:ALA:HB2	2.42	0.45
1:A:1092:ILE:O	1:A:1122:THR:OG1	2.34	0.45
1:B:1223:MET:HA	1:B:1226:THR:HG22	1.98	0.45
1:B:1396:ASP:O	1:B:1400:PRO:HD2	2.16	0.45
1:C:1354:LYS:HZ3	1:C:1405:PHE:HD1	1.63	0.45
1:D:1296:ASP:O	1:D:1366:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:HA	1:A:1127:MET:HB2	1.98	0.45
1:C:1331:ASP:CG	1:C:1343:LYS:HZ1	2.25	0.45
1:D:760:LEU:O	1:D:761:LEU:HG	2.16	0.45
1:A:339:ARG:NH2	1:A:946:ASN:HB2	2.31	0.45
1:B:135:GLN:HE22	1:B:148:GLN:HE21	1.65	0.45
1:B:1250:MET:SD	1:B:1256:PHE:HZ	2.40	0.45
1:B:31:ILE:HG12	1:B:1030:VAL:HB	1.98	0.45
1:B:239:LYS:HZ3	1:B:1275:LYS:NZ	2.12	0.45
1:B:281:ASP:OD1	1:B:988:ARG:NH1	2.44	0.45
1:B:807:ASN:O	1:B:864:SER:HB2	2.17	0.45
1:D:1081:PHE:CE2	1:D:1134:LEU:HD12	2.52	0.45
1:A:317:ASP:O	1:A:320:LYS:HB3	2.17	0.45
1:B:879:PHE:N	1:B:879:PHE:HD1	2.15	0.45
1:B:925:ARG:NH1	1:B:960:TYR:OH	2.50	0.45
1:C:49:LEU:CD2	1:C:64:LEU:HD13	2.45	0.45
1:C:687:PRO:HD2	1:C:735:ILE:O	2.17	0.45
1:D:232:TYR:CD2	1:D:996:MET:SD	3.10	0.45
1:D:1092:ILE:O	1:D:1122:THR:OG1	2.35	0.45
1:B:397:LEU:HD13	1:B:844:LEU:HD13	1.98	0.44
1:B:1036:LEU:HD21	1:B:1039:ILE:HG12	1.99	0.44
1:D:338:HIS:CD2	1:D:341:ASN:ND2	2.80	0.44
1:A:1323:PRO:CA	1:A:1368:ARG:HG3	2.47	0.44
1:B:1357:HIS:CE1	1:B:1404:GLN:HE22	2.35	0.44
1:B:1398:ASP:HA	1:B:1401:ASN:HB2	1.99	0.44
1:C:286:GLU:H	1:C:286:GLU:CD	2.25	0.44
1:C:1076:ALA:H	1:C:1376:ASP:CG	2.24	0.44
1:D:31:ILE:HD12	1:D:236:LEU:HD13	1.98	0.44
1:A:349:GLY:HA2	1:A:917:ASN:HB2	1.99	0.44
1:B:1247:ILE:H	1:B:1247:ILE:HG13	1.62	0.44
1:C:79:LYS:HZ2	1:C:972:GLU:CA	2.26	0.44
1:C:296:LYS:HZ3	1:C:326:GLY:CA	2.26	0.44
1:C:296:LYS:CD	1:C:326:GLY:HA2	2.42	0.44
1:D:995:GLY:C	1:D:996:MET:HG2	2.41	0.44
1:B:1200:ILE:HG13	1:B:1230:VAL:HG22	1.99	0.44
1:C:112:ALA:O	1:C:116:VAL:HG23	2.16	0.44
1:D:362:ASP:HA	1:D:365:ILE:HB	1.99	0.44
1:D:1295:LEU:HD21	1:D:1298:VAL:HG22	1.98	0.44
1:A:345:PHE:HD2	1:A:893:TRP:NE1	2.15	0.44
1:A:703:LEU:HD23	1:A:733:LEU:HD13	2.00	0.44
1:C:693:LYS:H	1:C:693:LYS:HZ2	1.61	0.44
1:D:316:GLN:HE21	1:D:961:ARG:NH1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.99	0.44
1:B:1215:LEU:HB3	1:B:1303:ALA:HB1	2.00	0.44
1:B:1382:TYR:HA	1:B:1385:LEU:CG	2.40	0.44
1:D:296:LYS:NZ	1:D:326:GLY:CA	2.78	0.44
1:D:1075:MET:SD	1:D:1379:ARG:CZ	3.06	0.44
1:D:1197:HIS:CE1	1:D:1231:LYS:HZ3	2.36	0.44
1:A:1214:MET:HB3	1:A:1304:ASP:HA	2.00	0.44
1:B:286:GLU:CD	1:B:286:GLU:H	2.26	0.44
1:B:296:LYS:CD	1:B:326:GLY:HA2	2.41	0.44
1:C:104:LYS:HD3	1:C:967:SER:HA	1.99	0.44
1:A:1206:ALA:HB1	1:A:1211:TYR:HB3	2.00	0.44
1:B:363:ARG:NH1	1:B:879:PHE:CE1	2.86	0.44
1:B:1115:PRO:HG3	1:B:1137:ARG:NE	2.32	0.44
1:C:760:LEU:O	1:C:761:LEU:HG	2.18	0.44
1:C:1105:LEU:CA	1:C:1138:LEU:HG	2.32	0.44
1:B:1378:LEU:HB3	1:B:1399:LEU:HD21	1.99	0.44
1:D:135:GLN:HE22	1:D:148:GLN:HE21	1.66	0.44
1:C:362:ASP:HA	1:C:365:ILE:HB	1.98	0.43
1:A:286:GLU:CD	1:A:286:GLU:H	2.26	0.43
1:B:387:LEU:HD13	1:B:862:LEU:HD23	1.99	0.43
1:B:1231:LYS:NZ	1:B:1233:TRP:CH2	2.78	0.43
1:B:1351:LEU:HA	1:B:1354:LYS:HZ1	1.82	0.43
1:C:29:PRO:HB2	1:C:986:VAL:O	2.18	0.43
1:C:56:ASN:OD1	1:C:58:THR:OG1	2.33	0.43
1:C:1058:GLN:HB3	1:C:1293:LEU:HD13	2.00	0.43
1:D:1061:LEU:HD11	1:D:1090:TYR:HB3	1.99	0.43
1:D:1121:ASN:C	1:D:1123:GLU:H	2.26	0.43
1:B:105:LEU:HD12	1:B:966:SER:HA	2.00	0.43
1:C:863:THR:O	1:C:866:THR:OG1	2.31	0.43
1:C:1115:PRO:HG3	1:C:1137:ARG:NE	2.34	0.43
1:D:1130:GLN:HE21	1:D:1130:GLN:N	2.16	0.43
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.54	0.43
1:B:49:LEU:CD2	1:B:64:LEU:HD13	2.43	0.43
1:B:113:THR:H	1:B:114:PRO:CD	2.30	0.43
1:B:1215:LEU:O	1:B:1219:MET:SD	2.75	0.43
1:C:961:ARG:NH2	1:C:983:PHE:CD2	2.86	0.43
1:C:1140:ARG:CZ	1:C:1145:GLU:HA	2.47	0.43
1:A:339:ARG:HH11	1:A:898:THR:HG21	1.82	0.43
1:A:1366:LEU:O	1:A:1370:ARG:HG3	2.19	0.43
1:B:1263:TYR:HB2	1:B:1290:LEU:HD12	2.00	0.43
1:C:925:ARG:HB2	1:C:960:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1354:LYS:NZ	1:C:1405:PHE:HD1	2.16	0.43
1:A:31:ILE:HA	1:A:1030:VAL:HB	1.99	0.43
1:A:243:TYR:O	1:A:244:ILE:CG1	2.65	0.43
1:A:341:ASN:HB2	1:A:893:TRP:CG	2.53	0.43
1:B:703:LEU:HD23	1:B:733:LEU:HD13	1.99	0.43
1:B:880:ASP:HB3	1:B:881:ASN:CA	2.40	0.43
1:B:988:ARG:HA	1:B:1018:ILE:HB	1.99	0.43
1:C:316:GLN:HB2	1:C:961:ARG:HD2	1.98	0.43
1:D:117:GLU:CA	1:D:120:TYR:HB2	2.41	0.43
1:D:687:PRO:HD2	1:D:735:ILE:O	2.18	0.43
1:A:928:ALA:HB1	1:A:962:TYR:HB2	2.01	0.43
1:A:1331:ASP:CB	1:A:1343:LYS:HZ1	2.27	0.43
1:C:693:LYS:NZ	1:C:693:LYS:N	2.58	0.43
1:C:1331:ASP:CB	1:C:1343:LYS:NZ	2.81	0.43
1:D:286:GLU:CD	1:D:286:GLU:H	2.26	0.43
1:D:1130:GLN:HE21	1:D:1130:GLN:H	1.67	0.43
1:A:204:LEU:HD12	1:A:209:LYS:HB2	1.99	0.43
1:B:1306:ILE:HD13	1:B:1457:TRP:HB3	2.00	0.43
1:B:1416:TRP:O	1:B:1433:THR:OG1	2.27	0.43
1:C:878:ILE:CG2	1:C:1044:HIS:CE1	2.93	0.43
1:C:1226:THR:HG21	1:C:1230:VAL:HG21	2.01	0.43
1:D:142:PHE:CE1	1:D:185:LEU:HB2	2.54	0.43
1:A:312:LEU:HA	1:A:315:THR:HG22	2.01	0.43
1:B:110:ARG:CZ	1:B:227:LEU:HD11	2.48	0.43
1:C:42:PRO:HB3	1:C:116:VAL:HG11	2.01	0.43
1:C:53:ALA:HB1	1:C:60:TYR:HB2	2.00	0.43
1:B:408:SER:HB2	1:B:655:ARG:NH2	2.34	0.43
1:B:1152:PRO:HA	1:B:1153:SER:HA	1.70	0.43
1:C:95:MET:HB3	1:C:100:LEU:HG	2.01	0.43
1:C:737:HIS:NE2	1:C:749:LEU:CD1	2.82	0.43
1:C:1130:GLN:N	1:C:1130:GLN:HE21	2.17	0.43
1:D:231:GLY:HA2	1:D:367:PRO:CG	2.49	0.43
1:D:281:ASP:O	1:D:987:PRO:HB3	2.18	0.43
1:D:806:LEU:HD23	1:D:832:GLU:HG2	2.01	0.43
1:D:988:ARG:HA	1:D:1018:ILE:HB	2.01	0.43
1:D:1058:GLN:HB3	1:D:1293:LEU:CD1	2.48	0.43
1:D:1107:SER:HB2	1:D:1120:ASP:CA	2.29	0.43
1:D:1331:ASP:CB	1:D:1343:LYS:NZ	2.81	0.43
1:D:1331:ASP:CG	1:D:1343:LYS:NZ	2.77	0.43
1:A:1115:PRO:HG3	1:A:1137:ARG:NE	2.34	0.42
1:C:105:LEU:HD12	1:C:105:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LEU:HD12	1:D:81:LEU:HD22	2.00	0.42
1:D:348:GLU:HB2	1:D:947:PRO:O	2.18	0.42
1:D:795:SER:HB3	1:D:797:MET:HE3	1.99	0.42
1:A:1323:PRO:HA	1:A:1368:ARG:HG3	2.00	0.42
1:B:686:VAL:O	1:B:688:VAL:HG23	2.20	0.42
1:B:1200:ILE:HB	1:B:1230:VAL:HG13	2.01	0.42
1:B:1361:LEU:HB3	1:B:1417:LEU:HD22	2.00	0.42
1:B:1394:ASN:HB2	1:B:1398:ASP:HB2	2.01	0.42
1:C:957:LYS:HZ3	1:C:957:LYS:N	2.17	0.42
1:D:840:VAL:HG12	1:D:844:LEU:HD22	2.00	0.42
1:A:821:LYS:HZ3	1:C:1270:ARG:HH12	1.65	0.42
1:A:1331:ASP:CG	1:A:1343:LYS:NZ	2.78	0.42
1:C:142:PHE:CE1	1:C:185:LEU:HB2	2.54	0.42
1:C:1333:ARG:HE	1:C:1424:SER:HA	1.85	0.42
1:D:339:ARG:HH12	1:D:946:ASN:CB	2.26	0.42
1:A:929:VAL:HG12	1:A:933:LEU:HD11	2.02	0.42
1:A:1055:ARG:HD3	1:A:1076:ALA:HB2	2.01	0.42
1:A:1368:ARG:HD2	1:A:1372:LEU:HD22	2.00	0.42
1:B:105:LEU:HB2	1:B:966:SER:HA	2.01	0.42
1:B:298:ALA:HB2	1:B:918:PRO:HG2	2.00	0.42
1:B:1280:TRP:HA	1:B:1283:LYS:CD	2.49	0.42
1:C:811:LEU:HD23	1:C:811:LEU:HA	1.93	0.42
1:A:42:PRO:HB3	1:A:116:VAL:HG11	2.01	0.42
1:A:355:LEU:HD11	1:A:910:ILE:HG23	2.00	0.42
1:A:1416:TRP:O	1:A:1433:THR:OG1	2.29	0.42
1:A:1450:ALA:HB1	1:A:1457:TRP:CD1	2.54	0.42
1:B:318:PHE:HB3	1:B:319:PRO:HD3	2.01	0.42
1:C:283:LYS:HA	1:C:284:PRO:HD3	1.93	0.42
1:C:917:ASN:OD1	1:C:947:PRO:HA	2.20	0.42
1:A:1218:MET:HB2	1:A:1303:ALA:O	2.19	0.42
1:A:1323:PRO:HB3	1:A:1368:ARG:HG3	2.02	0.42
1:B:142:PHE:CE1	1:B:185:LEU:HB2	2.55	0.42
1:B:737:HIS:NE2	1:B:749:LEU:CD1	2.82	0.42
1:B:1336:MET:HE2	1:B:1421:THR:HG22	2.01	0.42
1:A:110:ARG:HD3	1:A:227:LEU:HD21	2.02	0.42
1:A:142:PHE:CE1	1:A:185:LEU:HB2	2.54	0.42
1:B:760:LEU:O	1:B:761:LEU:HG	2.20	0.42
1:B:1319:LEU:HB2	1:B:1322:ALA:O	2.20	0.42
1:B:1403:MET:HB3	1:B:1407:ILE:HD12	2.02	0.42
1:C:317:ASP:OD1	1:C:961:ARG:NH2	2.52	0.42
1:C:760:LEU:HD23	1:C:763:PHE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1121:ASN:C	1:C:1123:GLU:H	2.28	0.42
1:C:1416:TRP:O	1:C:1433:THR:OG1	2.29	0.42
1:C:1450:ALA:HB1	1:C:1457:TRP:CD1	2.54	0.42
1:D:109:LEU:HD21	1:D:964:LEU:HD11	2.02	0.42
1:D:703:LEU:HD23	1:D:733:LEU:HD13	2.02	0.42
1:D:737:HIS:NE2	1:D:749:LEU:CD1	2.83	0.42
1:D:1335:GLU:HG2	1:D:1336:MET:SD	2.60	0.42
1:B:36:LYS:HD2	1:B:226:SER:HB3	2.00	0.42
1:B:302:MET:SD	1:B:897:TYR:O	2.78	0.42
1:B:1121:ASN:C	1:B:1123:GLU:H	2.27	0.42
1:B:1454:VAL:O	1:B:1454:VAL:HG12	2.20	0.42
1:C:1314:LEU:HD13	1:C:1416:TRP:CE2	2.54	0.42
1:D:1214:MET:HB3	1:D:1304:ASP:HA	2.01	0.42
1:D:1218:MET:HB2	1:D:1303:ALA:O	2.20	0.42
1:D:1225:HIS:HD1	1:D:1308:ARG:HA	1.84	0.42
1:D:1333:ARG:HE	1:D:1424:SER:HA	1.84	0.42
1:D:1450:ALA:HB1	1:D:1457:TRP:CD1	2.55	0.42
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	2.02	0.42
1:B:1130:GLN:HE21	1:B:1130:GLN:N	2.18	0.42
1:B:1336:MET:SD	1:B:1421:THR:O	2.78	0.42
1:C:669:VAL:HB	1:C:868:LEU:HD21	2.00	0.42
1:C:861:LYS:O	1:C:865:VAL:HG23	2.20	0.42
1:D:31:ILE:HG12	1:D:1030:VAL:HB	2.00	0.42
1:D:281:ASP:OD1	1:D:988:ARG:NH1	2.45	0.42
1:B:281:ASP:O	1:B:987:PRO:HB3	2.20	0.42
1:C:44:TYR:HB3	1:C:81:LEU:HD13	2.02	0.42
1:C:204:LEU:HD12	1:C:209:LYS:HB2	2.02	0.42
1:C:1218:MET:HB2	1:C:1303:ALA:O	2.20	0.42
1:D:999:PRO:HA	1:D:1000:PRO:HD3	1.93	0.42
1:D:1200:ILE:HD12	1:D:1230:VAL:HG22	2.00	0.42
1:A:353:LEU:HG	1:A:360:LEU:HD13	2.00	0.41
1:A:1061:LEU:HD23	1:A:1069:PHE:HD2	1.84	0.41
1:A:1105:LEU:O	1:A:1105:LEU:HG	2.20	0.41
1:B:243:TYR:O	1:B:244:ILE:HG13	2.19	0.41
1:B:811:LEU:HD23	1:B:811:LEU:HA	1.92	0.41
1:C:958:ARG:HH21	1:C:1273:LYS:NZ	2.18	0.41
1:C:1084:LYS:H	1:C:1084:LYS:HG3	1.69	0.41
1:D:367:PRO:HB2	1:D:368:PHE:H	1.74	0.41
1:B:204:LEU:HD12	1:B:209:LYS:HB2	2.02	0.41
1:B:1005:THR:HB	1:B:1237:GLN:HA	2.01	0.41
1:C:686:VAL:O	1:C:688:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1213:ARG:HH22	1:C:1451:ARG:NH1	2.18	0.41
1:D:317:ASP:CG	1:D:320:LYS:HD3	2.45	0.41
1:A:1200:ILE:HD12	1:A:1230:VAL:HG22	2.02	0.41
1:B:42:PRO:HG2	1:B:113:THR:HG22	2.02	0.41
1:B:1457:TRP:HA	1:B:1460:TYR:CD2	2.55	0.41
1:C:319:PRO:HD2	1:C:959:PHE:CE1	2.54	0.41
1:A:988:ARG:HB3	1:A:1019:LYS:HB2	2.02	0.41
1:A:1225:HIS:HD1	1:A:1308:ARG:HA	1.85	0.41
1:B:362:ASP:HA	1:B:365:ILE:HB	2.01	0.41
1:B:1205:VAL:CG1	1:B:1235:ILE:HG13	2.51	0.41
1:C:1209:HIS:CE1	1:C:1242:SER:HB2	2.55	0.41
1:A:760:LEU:O	1:A:761:LEU:HG	2.20	0.41
1:B:1105:LEU:HG	1:B:1105:LEU:O	2.20	0.41
1:C:235:GLU:HG2	1:C:995:GLY:O	2.20	0.41
1:C:284:PRO:HB2	1:C:323:ASN:HB2	2.02	0.41
1:C:296:LYS:NZ	1:C:326:GLY:CA	2.80	0.41
1:C:1105:LEU:O	1:C:1105:LEU:HG	2.20	0.41
1:C:1119:ASP:C	1:C:1121:ASN:H	2.28	0.41
1:A:338:HIS:C	1:A:340:GLY:H	2.29	0.41
1:A:686:VAL:O	1:A:688:VAL:HG23	2.20	0.41
1:A:1121:ASN:C	1:A:1123:GLU:H	2.29	0.41
1:A:1428:LEU:HA	1:A:1431:ALA:HB2	2.03	0.41
1:C:243:TYR:O	1:C:285:LEU:HG	2.21	0.41
1:C:363:ARG:C	1:C:365:ILE:H	2.28	0.41
1:A:737:HIS:NE2	1:A:749:LEU:CD1	2.83	0.41
1:A:1140:ARG:CZ	1:A:1145:GLU:HA	2.50	0.41
1:B:239:LYS:HZ3	1:B:1275:LYS:HZ2	1.68	0.41
1:B:1119:ASP:C	1:B:1121:ASN:H	2.29	0.41
1:B:1140:ARG:CZ	1:B:1145:GLU:HA	2.51	0.41
1:C:1059:LEU:HD11	1:C:1094:LEU:HD23	2.02	0.41
1:A:48:LEU:CD2	1:A:82:TYR:HA	2.50	0.41
1:A:1305:GLN:HG2	1:A:1435:ASP:HA	2.02	0.41
1:B:296:LYS:NZ	1:B:326:GLY:CA	2.82	0.41
1:B:899:SER:HB2	1:B:944:PHE:CE2	2.56	0.41
1:B:1098:ARG:NE	1:B:1152:PRO:HB3	2.36	0.41
1:B:1215:LEU:O	1:B:1218:MET:HB3	2.21	0.41
1:B:1420:GLU:HB2	1:B:1453:GLN:OE1	2.21	0.41
1:C:1203:PHE:HB3	1:C:1298:VAL:CG1	2.51	0.41
1:C:1223:MET:HG3	1:C:1254:TYR:HB3	2.03	0.41
1:D:204:LEU:HD12	1:D:209:LYS:HB2	2.01	0.41
1:D:961:ARG:CD	1:D:983:PHE:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1059:LEU:HD11	1:D:1094:LEU:HD23	2.03	0.41
1:D:1203:PHE:HB3	1:D:1298:VAL:HG11	2.03	0.41
1:A:95:MET:HB3	1:A:100:LEU:HG	2.02	0.41
1:A:345:PHE:C	1:A:345:PHE:HD1	2.28	0.41
1:A:399:GLY:HA2	1:A:886:ARG:CB	2.50	0.41
1:B:243:TYR:O	1:B:285:LEU:HG	2.21	0.41
1:B:748:VAL:O	1:B:752:ARG:HG2	2.21	0.41
1:B:975:LYS:HE3	1:B:976:VAL:HB	2.03	0.41
1:C:692:SER:CA	1:C:693:LYS:NZ	2.78	0.41
1:D:1213:ARG:HH22	1:D:1451:ARG:NH1	2.19	0.41
1:D:1404:GLN:HA	1:D:1407:ILE:O	2.19	0.41
1:A:400:HIS:CD2	1:A:402:GLU:OE2	2.74	0.41
1:A:806:LEU:HD23	1:A:832:GLU:HG2	2.03	0.41
1:A:1319:LEU:HD12	1:A:1365:ASP:HB2	2.03	0.41
1:A:1404:GLN:HA	1:A:1407:ILE:O	2.21	0.41
1:B:878:ILE:HD13	1:B:1133:THR:HG21	2.03	0.41
1:C:31:ILE:HA	1:C:1030:VAL:HB	2.03	0.41
1:C:1108:VAL:HG11	1:C:1124:VAL:CG1	2.51	0.41
1:C:1342:TRP:CD1	1:C:1343:LYS:HG3	2.56	0.41
1:D:52:ALA:HB1	1:D:89:LEU:CD2	2.50	0.41
1:D:349:GLY:HA2	1:D:917:ASN:CB	2.51	0.41
1:A:1342:TRP:CD1	1:A:1343:LYS:HG3	2.56	0.40
1:B:709:LEU:H	1:B:737:HIS:HD1	1.70	0.40
1:B:1326:PHE:HB2	1:B:1357:HIS:CD2	2.55	0.40
1:B:1333:ARG:HB2	1:B:1422:TRP:O	2.21	0.40
1:B:1350:TYR:HD2	1:D:771:THR:HG22	1.86	0.40
1:C:969:SER:HB2	1:C:977:LYS:HB3	2.03	0.40
1:C:1404:GLN:HA	1:C:1407:ILE:O	2.21	0.40
1:D:31:ILE:HA	1:D:1030:VAL:HB	2.03	0.40
1:D:1105:LEU:HG	1:D:1105:LEU:O	2.22	0.40
1:A:341:ASN:HD22	1:A:341:ASN:C	2.29	0.40
1:A:1314:LEU:HD11	1:A:1412:LEU:HD13	2.02	0.40
1:A:1460:TYR:O	1:A:1464:ILE:HG12	2.21	0.40
1:B:946:ASN:HA	1:B:947:PRO:HD3	1.87	0.40
1:C:281:ASP:O	1:C:987:PRO:HB3	2.21	0.40
1:D:748:VAL:O	1:D:752:ARG:HG2	2.22	0.40
1:D:1314:LEU:HD13	1:D:1416:TRP:CE2	2.56	0.40
1:A:1234:PHE:CD1	1:A:1260:MET:SD	3.10	0.40
1:B:37:ALA:O	1:B:226:SER:OG	2.38	0.40
1:B:1458:THR:O	1:B:1461:ASP:HB3	2.21	0.40
1:C:338:HIS:CD2	1:C:341:ASN:ND2	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:899:SER:HB2	1:C:944:PHE:CE2	2.56	0.40
1:C:1200:ILE:HD12	1:C:1230:VAL:HG22	2.03	0.40
1:C:1223:MET:HA	1:C:1226:THR:HG22	2.03	0.40
1:D:760:LEU:HD23	1:D:763:PHE:HE2	1.85	0.40
1:D:1090:TYR:HB2	1:D:1124:VAL:HG23	2.03	0.40
1:A:102:ALA:HB1	1:A:374:LEU:HD21	2.03	0.40
1:A:760:LEU:HD23	1:A:763:PHE:HE2	1.86	0.40
1:A:899:SER:HB2	1:A:944:PHE:CE2	2.57	0.40
1:B:998:VAL:HG21	1:B:1004:VAL:HG21	2.02	0.40
1:C:664:LYS:HA	1:C:664:LYS:HD3	1.92	0.40
1:C:1090:TYR:HB2	1:C:1124:VAL:O	2.20	0.40
1:D:312:LEU:HD13	1:D:928:ALA:HA	2.04	0.40
1:D:1416:TRP:CD2	1:D:1432:ARG:HD2	2.57	0.40
1:A:101:SER:OG	1:A:936:LEU:HA	2.22	0.40
1:B:48:LEU:HD13	1:B:85:PHE:CD1	2.56	0.40
1:B:1221:SER:O	1:B:1225:HIS:HB2	2.22	0.40
1:B:1319:LEU:HD13	1:B:1368:ARG:HB2	2.02	0.40
1:C:703:LEU:HD23	1:C:733:LEU:HD13	2.03	0.40
1:C:1331:ASP:CG	1:C:1343:LYS:NZ	2.79	0.40
1:D:44:TYR:HB3	1:D:81:LEU:HD13	2.04	0.40
1:D:1223:MET:HA	1:D:1226:THR:HG22	2.03	0.40
1:D:1263:TYR:HB2	1:D:1290:LEU:HD12	2.03	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	1101/1260 (87%)	1009 (92%)	78 (7%)	14 (1%)	9	41
1	B	1110/1260 (88%)	947 (85%)	134 (12%)	29 (3%)	4	25
1	C	1105/1260 (88%)	991 (90%)	98 (9%)	16 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1115/1260 (88%)	987 (88%)	100 (9%)	28 (2%)	4	25
All	All	4431/5040 (88%)	3934 (89%)	410 (9%)	87 (2%)	6	30

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ALA
1	A	873	ASP
1	A	874	LEU
1	A	876	GLN
1	A	883	PRO
1	A	1303	ALA
1	B	332	ALA
1	B	367	PRO
1	B	882	ALA
1	B	1199	GLU
1	B	1225	HIS
1	B	1236	GLU
1	B	1237	GLN
1	B	1275	LYS
1	B	1285	LEU
1	B	1388	ASP
1	C	332	ALA
1	C	367	PRO
1	C	1303	ALA
1	D	332	ALA
1	D	367	PRO
1	D	655	ARG
1	D	656	ASN
1	D	881	ASN
1	D	1303	ALA
1	D	1437	CYS
1	A	244	ILE
1	A	884	THR
1	A	1345	GLY
1	A	1437	CYS
1	B	661	PRO
1	B	883	PRO
1	B	1079	GLY
1	B	1205	VAL
1	B	1206	ALA
1	B	1255	GLY

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Mol	Chain	Res	Type
1	C	1127	MET
1	C	1345	GLY
1	C	1368	ARG
1	C	1437	CYS
1	C	1439	ASN
1	D	55	ASP
1	D	244	ILE
1	D	287	LYS
1	D	1345	GLY
1	D	1439	ASN
1	A	287	LYS
1	B	244	ILE
1	B	287	LYS
1	B	407	LYS
1	B	879	PHE
1	B	1303	ALA
1	B	1396	ASP
1	C	244	ILE
1	C	287	LYS
1	C	407	LYS
1	C	875	PRO
1	D	56	ASN
1	D	407	LYS
1	D	660	PHE
1	D	872	SER
1	D	1373	ALA
1	B	56	ASN
1	B	113	THR
1	B	1427	THR
1	C	1440	PRO
1	D	658	LEU
1	D	1368	ARG
1	D	1440	PRO
1	A	162	LYS
1	A	880	ASP
1	B	162	LYS
1	B	218	ARG
1	B	975	LYS
1	C	54	SER
1	D	162	LYS
1	D	664	LYS
1	D	1377	ARG

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Mol	Chain	Res	Type
1	C	162	LYS
1	D	882	ALA
1	D	971	ASP
1	D	1472	ARG
1	D	366	GLN
1	B	366	GLN
1	A	307	PRO
1	C	967	SER
1	D	113	THR

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	965/1088 (89%)	884 (92%)	81 (8%)	10	29
1	B	974/1088 (90%)	838 (86%)	136 (14%)	3	13
1	C	967/1088 (89%)	873 (90%)	94 (10%)	8	24
1	D	977/1088 (90%)	884 (90%)	93 (10%)	8	25
All	All	3883/4352 (89%)	3479 (90%)	404 (10%)	7	22

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	145	ASP
1	A	148	GLN
1	A	192	LYS
1	A	194	PHE
1	A	204	LEU
1	A	222	HIS
1	A	226	SER
1	A	227	LEU
1	A	238	LEU
1	A	239	LYS
1	A	242	ASP

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Mol	Chain	Res	Type
1	A	286	GLU
1	A	308	PHE
1	A	318	PHE
1	A	338	HIS
1	A	341	ASN
1	A	342	ARG
1	A	350	SER
1	A	351	ASN
1	A	359	HIS
1	A	360	LEU
1	A	361	ILE
1	A	362	ASP
1	A	363	ARG
1	A	366	GLN
1	A	372	ASP
1	A	374	LEU
1	A	376	ARG
1	A	377	GLU
1	A	380	LEU
1	A	408	SER
1	A	662	GLU
1	A	664	LYS
1	A	666	GLU
1	A	670	LEU
1	A	680	HIS
1	A	693	LYS
1	A	754	LYS
1	A	758	ASP
1	A	798	LYS
1	A	802	ASN
1	A	820	PHE
1	A	838	LEU
1	A	847	LEU
1	A	851	ASP
1	A	874	LEU
1	A	946	ASN
1	A	952	GLU
1	A	972	GLU
1	A	975	LYS
1	A	1003	LEU
1	A	1005	THR
1	A	1007	LYS

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Mol	Chain	Res	Type
1	A	1010	VAL
1	A	1013	LEU
1	A	1021	ILE
1	A	1024	LYS
1	A	1029	HIS
1	A	1042	GLU
1	A	1046	ARG
1	A	1048	ILE
1	A	1052	HIS
1	A	1084	LYS
1	A	1096	GLU
1	A	1102	ILE
1	A	1105	LEU
1	A	1127	MET
1	A	1145	GLU
1	A	1151	GLU
1	A	1203	PHE
1	A	1209	HIS
1	A	1211	TYR
1	A	1247	ILE
1	A	1298	VAL
1	A	1331	ASP
1	A	1335	GLU
1	A	1344	THR
1	A	1395	LEU
1	A	1420	GLU
1	A	1437	CYS
1	B	46	VAL
1	B	54	SER
1	B	81	LEU
1	B	82	TYR
1	B	86	LEU
1	B	103	PHE
1	B	121	GLN
1	B	145	ASP
1	B	148	GLN
1	B	192	LYS
1	B	194	PHE
1	B	204	LEU
1	B	222	HIS
1	B	236	LEU
1	B	242	ASP

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Mol	Chain	Res	Type
1	B	243	TYR
1	B	286	GLU
1	B	293	LEU
1	B	295	MET
1	B	299	SER
1	B	306	LYS
1	B	308	PHE
1	B	315	THR
1	B	317	ASP
1	B	322	SER
1	B	338	HIS
1	B	339	ARG
1	B	341	ASN
1	B	342	ARG
1	B	353	LEU
1	B	359	HIS
1	B	377	GLU
1	B	380	LEU
1	B	385	LEU
1	B	658	LEU
1	B	664	LYS
1	B	666	GLU
1	B	670	LEU
1	B	693	LYS
1	B	742	THR
1	B	754	LYS
1	B	758	ASP
1	B	798	LYS
1	B	802	ASN
1	B	820	PHE
1	B	838	LEU
1	B	847	LEU
1	B	851	ASP
1	B	865	VAL
1	B	878	ILE
1	B	879	PHE
1	B	946	ASN
1	B	960	TYR
1	B	972	GLU
1	B	975	LYS
1	B	991	LEU
1	B	998	VAL

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Mol	Chain	Res	Type
1	B	1003	LEU
1	B	1005	THR
1	B	1007	LYS
1	B	1010	VAL
1	B	1013	LEU
1	B	1019	LYS
1	B	1029	HIS
1	B	1046	ARG
1	B	1048	ILE
1	B	1052	HIS
1	B	1059	LEU
1	B	1072	THR
1	B	1075	MET
1	B	1084	LYS
1	B	1089	VAL
1	B	1096	GLU
1	B	1102	ILE
1	B	1105	LEU
1	B	1107	SER
1	B	1126	LEU
1	B	1127	MET
1	B	1130	GLN
1	B	1145	GLU
1	B	1151	GLU
1	B	1197	HIS
1	B	1202	ILE
1	B	1205	VAL
1	B	1207	SER
1	B	1216	ASN
1	B	1219	MET
1	B	1226	THR
1	B	1235	ILE
1	B	1236	GLU
1	B	1237	GLN
1	B	1238	PHE
1	B	1244	LYS
1	B	1247	ILE
1	B	1250	MET
1	B	1254	TYR
1	B	1261	VAL
1	B	1262	THR
1	B	1270	ARG

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Mol	Chain	Res	Type
1	B	1273	LYS
1	B	1276	GLN
1	B	1280	TRP
1	B	1285	LEU
1	B	1286	PHE
1	B	1295	LEU
1	B	1296	ASP
1	B	1297	LYS
1	B	1298	VAL
1	B	1301	VAL
1	B	1302	ASP
1	B	1305	GLN
1	B	1306	ILE
1	B	1309	THR
1	B	1311	MET
1	B	1312	TYR
1	B	1313	ASP
1	B	1316	GLU
1	B	1324	TYR
1	B	1330	CYS
1	B	1331	ASP
1	B	1333	ARG
1	B	1344	THR
1	B	1364	VAL
1	B	1365	ASP
1	B	1377	ARG
1	B	1390	ASN
1	B	1395	LEU
1	B	1397	GLN
1	B	1398	ASP
1	B	1403	MET
1	B	1409	ILE
1	B	1412	LEU
1	B	1421	THR
1	B	1425	ASP
1	B	1447	LEU
1	B	1467	LEU
1	C	51	THR
1	C	54	SER
1	C	86	LEU
1	C	103	PHE
1	C	107	LEU

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Mol	Chain	Res	Type
1	C	145	ASP
1	C	148	GLN
1	C	192	LYS
1	C	194	PHE
1	C	204	LEU
1	C	239	LYS
1	C	242	ASP
1	C	243	TYR
1	C	286	GLU
1	C	295	MET
1	C	299	SER
1	C	306	LYS
1	C	308	PHE
1	C	315	THR
1	C	338	HIS
1	C	339	ARG
1	C	341	ASN
1	C	342	ARG
1	C	353	LEU
1	C	359	HIS
1	C	370	LEU
1	C	377	GLU
1	C	378	ARG
1	C	380	LEU
1	C	385	LEU
1	C	407	LYS
1	C	664	LYS
1	C	666	GLU
1	C	670	LEU
1	C	680	HIS
1	C	693	LYS
1	C	742	THR
1	C	754	LYS
1	C	758	ASP
1	C	798	LYS
1	C	802	ASN
1	C	820	PHE
1	C	838	LEU
1	C	844	LEU
1	C	847	LEU
1	C	851	ASP
1	C	862	LEU

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Mol	Chain	Res	Type
1	C	886	ARG
1	C	937	GLU
1	C	946	ASN
1	C	957	LYS
1	C	961	ARG
1	C	966	SER
1	C	972	GLU
1	C	975	LYS
1	C	979	LEU
1	C	991	LEU
1	C	993	VAL
1	C	998	VAL
1	C	1003	LEU
1	C	1007	LYS
1	C	1010	VAL
1	C	1013	LEU
1	C	1016	LEU
1	C	1018	ILE
1	C	1021	ILE
1	C	1029	HIS
1	C	1044	HIS
1	C	1046	ARG
1	C	1048	ILE
1	C	1052	HIS
1	C	1059	LEU
1	C	1072	THR
1	C	1084	LYS
1	C	1089	VAL
1	C	1096	GLU
1	C	1102	ILE
1	C	1105	LEU
1	C	1107	SER
1	C	1126	LEU
1	C	1127	MET
1	C	1130	GLN
1	C	1145	GLU
1	C	1203	PHE
1	C	1209	HIS
1	C	1247	ILE
1	C	1264	LYS
1	C	1298	VAL
1	C	1331	ASP

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Mol	Chain	Res	Type
1	C	1344	THR
1	C	1376	ASP
1	C	1395	LEU
1	C	1420	GLU
1	C	1437	CYS
1	D	44	TYR
1	D	47	GLU
1	D	81	LEU
1	D	86	LEU
1	D	108	SER
1	D	121	GLN
1	D	145	ASP
1	D	148	GLN
1	D	192	LYS
1	D	194	PHE
1	D	204	LEU
1	D	242	ASP
1	D	243	TYR
1	D	286	GLU
1	D	293	LEU
1	D	295	MET
1	D	299	SER
1	D	308	PHE
1	D	315	THR
1	D	322	SER
1	D	328	GLN
1	D	338	HIS
1	D	339	ARG
1	D	341	ASN
1	D	342	ARG
1	D	353	LEU
1	D	359	HIS
1	D	363	ARG
1	D	377	GLU
1	D	380	LEU
1	D	385	LEU
1	D	654	ARG
1	D	659	ILE
1	D	666	GLU
1	D	670	LEU
1	D	693	LYS
1	D	742	THR

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Mol	Chain	Res	Type
1	D	754	LYS
1	D	758	ASP
1	D	798	LYS
1	D	802	ASN
1	D	820	PHE
1	D	838	LEU
1	D	844	LEU
1	D	851	ASP
1	D	864	SER
1	D	865	VAL
1	D	871	ILE
1	D	881	ASN
1	D	946	ASN
1	D	959	PHE
1	D	960	TYR
1	D	964	LEU
1	D	972	GLU
1	D	989	GLU
1	D	991	LEU
1	D	996	MET
1	D	998	VAL
1	D	1003	LEU
1	D	1005	THR
1	D	1007	LYS
1	D	1010	VAL
1	D	1013	LEU
1	D	1016	LEU
1	D	1029	HIS
1	D	1046	ARG
1	D	1048	ILE
1	D	1052	HIS
1	D	1059	LEU
1	D	1072	THR
1	D	1075	MET
1	D	1084	LYS
1	D	1089	VAL
1	D	1096	GLU
1	D	1102	ILE
1	D	1105	LEU
1	D	1107	SER
1	D	1126	LEU
1	D	1130	GLN

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Mol	Chain	Res	Type
1	D	1145	GLU
1	D	1203	PHE
1	D	1209	HIS
1	D	1247	ILE
1	D	1264	LYS
1	D	1298	VAL
1	D	1331	ASP
1	D	1344	THR
1	D	1365	ASP
1	D	1370	ARG
1	D	1378	LEU
1	D	1395	LEU
1	D	1420	GLU
1	D	1437	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	316	GLN
1	A	341	ASN
1	A	364	GLN
1	A	392	GLN
1	A	715	GLN
1	A	728	ASN
1	A	738	ASN
1	A	894	ASN
1	A	917	ASN
1	A	1029	HIS
1	A	1086	ASN
1	A	1197	HIS
1	A	1201	ASN
1	A	1216	ASN
1	A	1267	HIS
1	A	1367	GLN
1	A	1402	HIS
1	A	1438	ASN
1	B	135	GLN
1	B	338	HIS
1	B	392	GLN
1	B	400	HIS
1	B	715	GLN

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Mol	Chain	Res	Type
1	B	728	ASN
1	B	738	ASN
1	B	876	GLN
1	B	946	ASN
1	B	1029	HIS
1	B	1044	HIS
1	B	1077	ASN
1	B	1197	HIS
1	B	1216	ASN
1	B	1224	HIS
1	B	1237	GLN
1	B	1267	HIS
1	B	1380	GLN
1	B	1383	HIS
1	B	1404	GLN
1	C	148	GLN
1	C	338	HIS
1	C	366	GLN
1	C	392	GLN
1	C	400	HIS
1	C	715	GLN
1	C	728	ASN
1	C	738	ASN
1	C	924	GLN
1	C	946	ASN
1	C	1029	HIS
1	C	1044	HIS
1	C	1130	GLN
1	C	1197	HIS
1	C	1201	ASN
1	C	1216	ASN
1	C	1237	GLN
1	D	135	GLN
1	D	316	GLN
1	D	338	HIS
1	D	392	GLN
1	D	400	HIS
1	D	715	GLN
1	D	728	ASN
1	D	738	ASN
1	D	876	GLN
1	D	881	ASN

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Mol	Chain	Res	Type
1	D	924	GLN
1	D	946	ASN
1	D	1029	HIS
1	D	1038	HIS
1	D	1044	HIS
1	D	1082	GLN
1	D	1197	HIS
1	D	1201	ASN
1	D	1267	HIS
1	D	1367	GLN
1	D	1383	HIS
1	D	1402	HIS
1	D	1438	ASN

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 ⓘ

15 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	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.31	0	17,19,21	1.14	2 (11%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	2.56	3 (17%)
2	BMA	E	3	2	11,11,12	0.41	0	15,15,17	0.97	1 (6%)
2	MAN	E	4	2	11,11,12	0.93	0	15,15,17	1.89	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	E	5	2	11,11,12	0.79	0	15,15,17	1.85	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	1.21	2 (11%)
3	NAG	F	2	3	14,14,15	0.36	0	17,19,21	1.13	1 (5%)
3	BMA	F	3	3	11,11,12	0.32	0	15,15,17	0.49	0
4	NAG	G	1	4,1	14,14,15	0.29	0	17,19,21	1.08	2 (11%)
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	1.58	4 (23%)
4	BMA	G	3	4	11,11,12	0.35	0	15,15,17	0.91	1 (6%)
4	MAN	G	4	4	11,11,12	0.74	0	15,15,17	1.31	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.29	0	17,19,21	1.07	2 (11%)
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	1.07	2 (11%)
3	BMA	H	3	3	11,11,12	0.30	0	15,15,17	0.40	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
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	1/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-C2-N2	6.24	120.27	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	6.16	120.44	112.19
2	E	2	NAG	O5-C1-C2	-5.94	102.10	111.29
2	E	5	MAN	C1-O5-C5	5.93	120.13	112.19
2	E	2	NAG	C1-O5-C5	5.03	118.93	112.19
4	G	2	NAG	C1-C2-N2	4.06	116.83	110.43
3	F	1	NAG	O5-C1-C2	-3.87	105.30	111.29
3	F	2	NAG	C1-C2-N2	3.78	116.39	110.43
4	G	4	MAN	C1-O5-C5	3.70	117.15	112.19
2	E	1	NAG	O5-C1-C2	-3.40	106.04	111.29
3	H	2	NAG	C1-C2-N2	3.37	115.74	110.43
4	G	3	BMA	C1-O5-C5	3.26	116.55	112.19
3	H	1	NAG	O5-C1-C2	-3.09	106.51	111.29
2	E	5	MAN	C1-C2-C3	3.01	114.03	109.64
4	G	1	NAG	O5-C1-C2	-2.91	106.79	111.29
4	G	2	NAG	C1-O5-C5	2.82	115.97	112.19
2	E	4	MAN	C1-C2-C3	2.80	113.72	109.64
4	G	1	NAG	C1-O5-C5	2.70	115.81	112.19
3	F	1	NAG	C1-O5-C5	2.65	115.73	112.19
3	H	1	NAG	C1-O5-C5	2.64	115.73	112.19
4	G	2	NAG	C2-N2-C7	2.63	126.42	122.90
2	E	1	NAG	C1-O5-C5	2.55	115.61	112.19
4	G	2	NAG	O5-C1-C2	-2.55	107.35	111.29
2	E	3	BMA	O3-C3-C4	2.40	116.04	110.38
4	G	4	MAN	C1-C2-C3	2.35	113.06	109.64
3	H	2	NAG	C2-N2-C7	2.16	125.80	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7

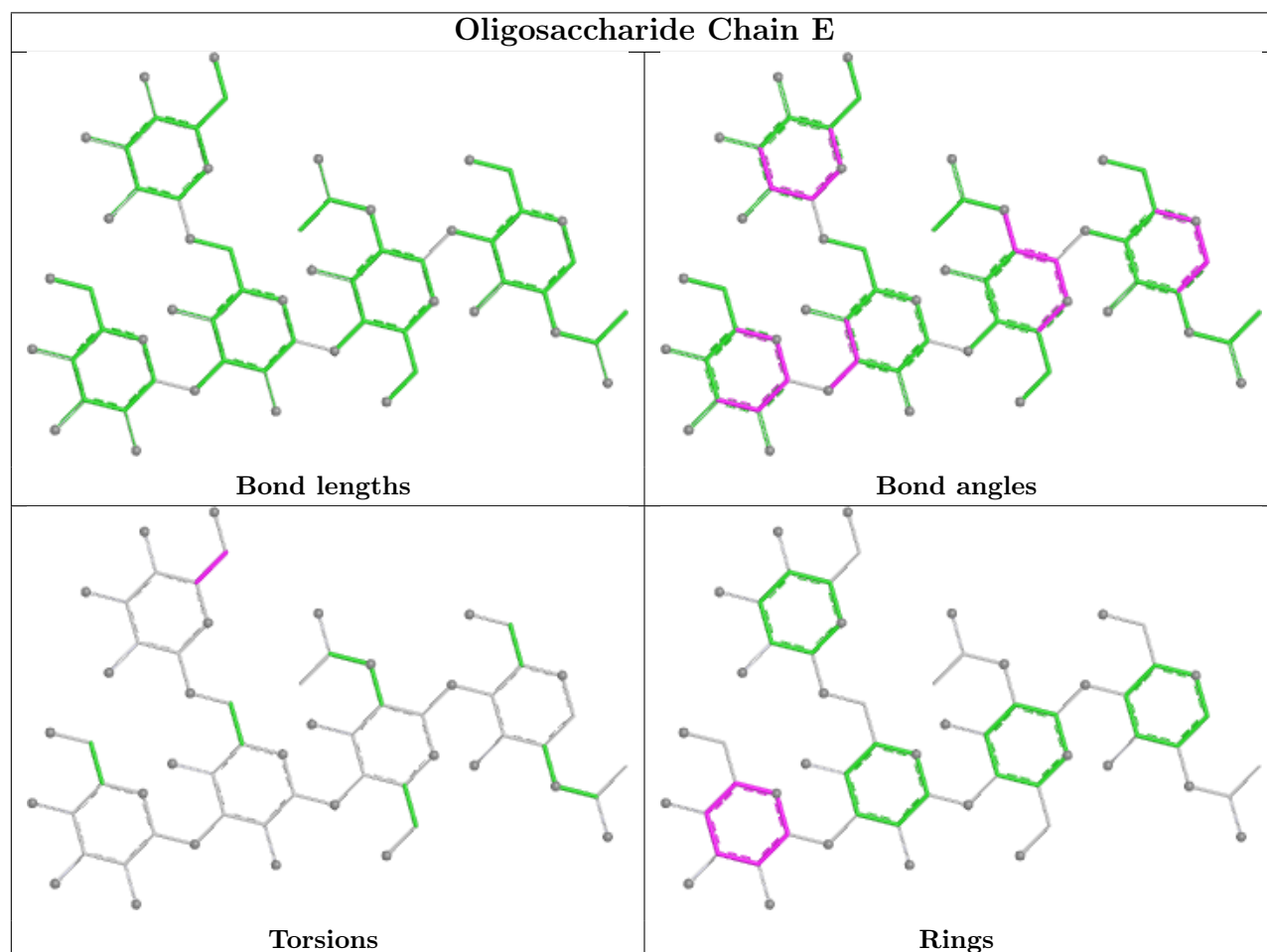
All (1) ring outliers are listed below:

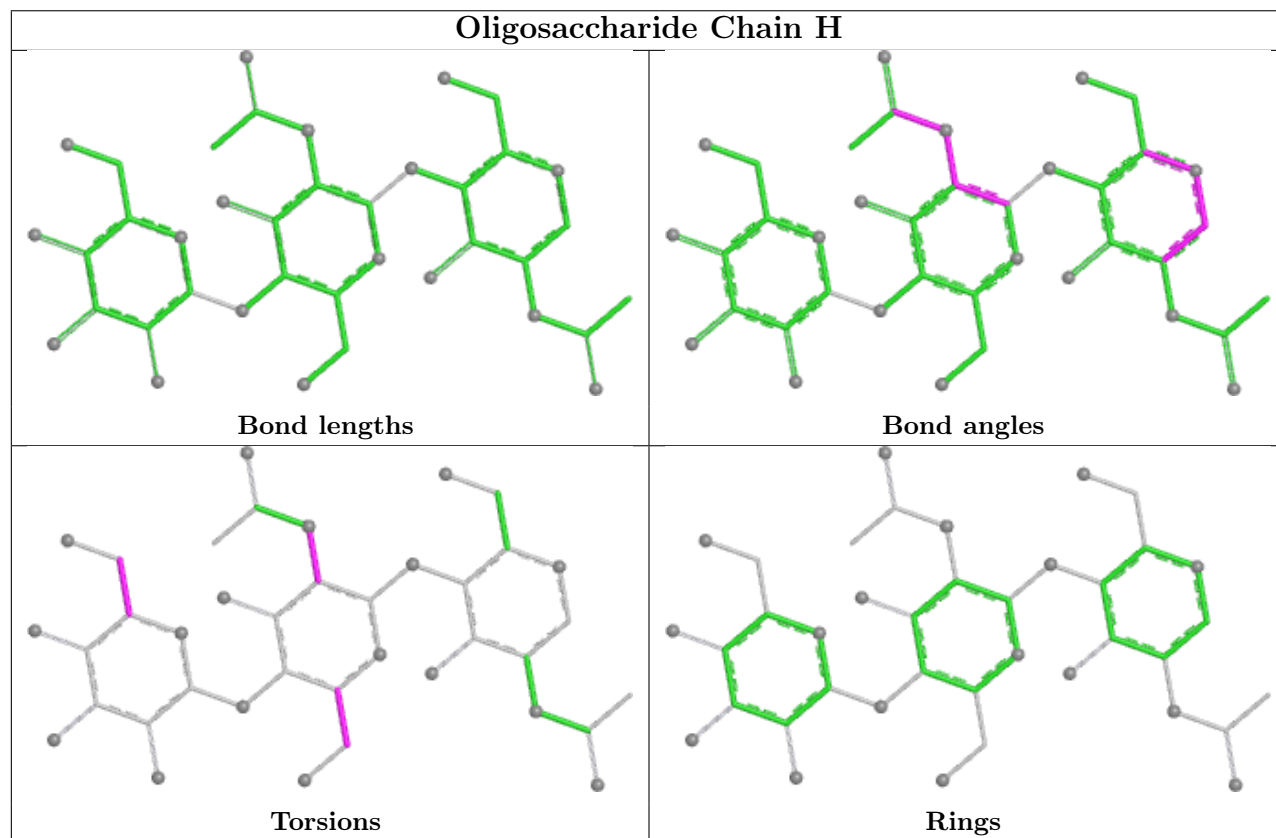
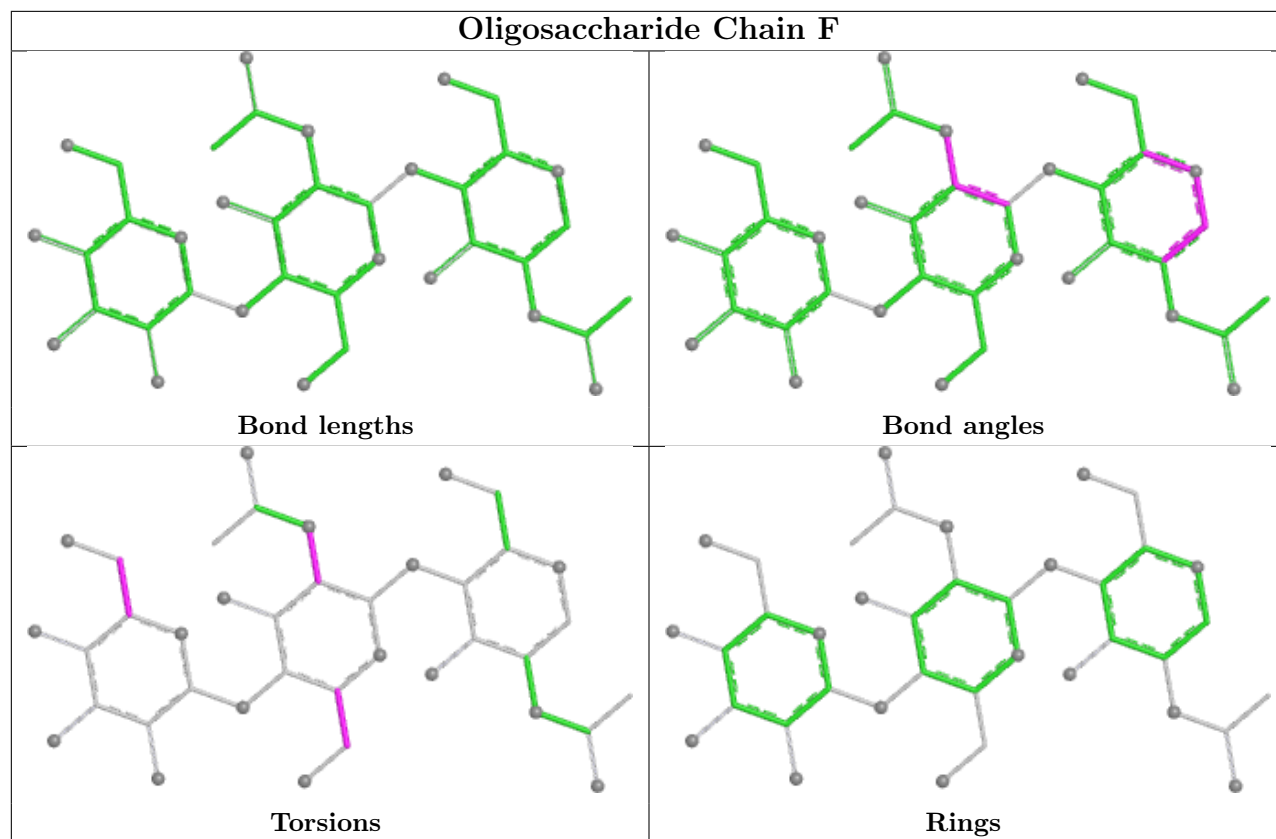
Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C1-C2-C3-C4-C5-O5

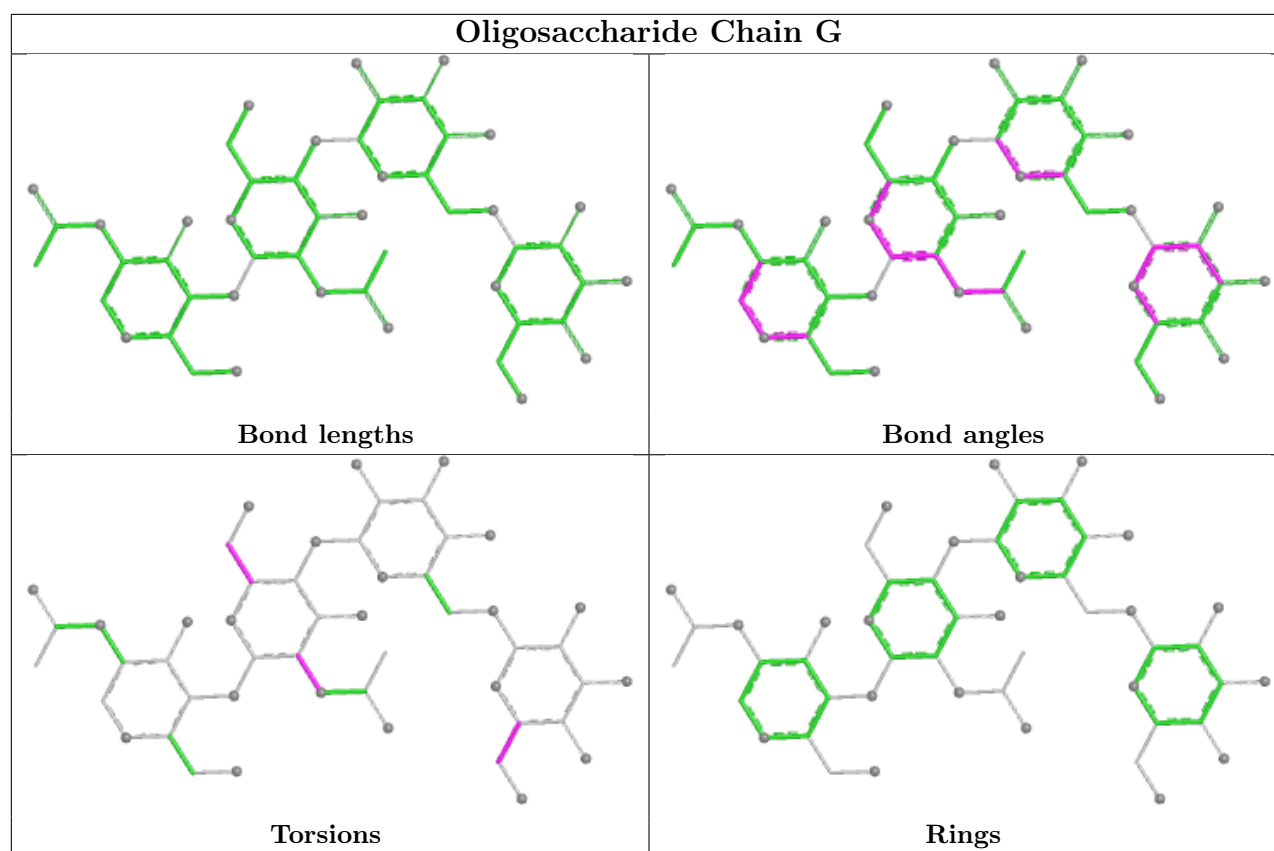
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	4	0
2	E	1	NAG	4	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
5	NAG	A	1602	1	14,14,15	0.30	0	17,19,21	0.80	1 (5%)
5	NAG	B	1602	1	14,14,15	0.37	0	17,19,21	1.20	1 (5%)
5	NAG	B	1603	1	14,14,15	0.39	0	17,19,21	1.02	2 (11%)
5	NAG	D	1601	-	14,14,15	0.32	0	17,19,21	0.68	0
5	NAG	A	1601	-	14,14,15	0.36	0	17,19,21	0.70	0
5	NAG	C	1607	1	14,14,15	0.30	0	17,19,21	0.58	0
5	NAG	C	1606	1	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
5	NAG	C	1601	-	14,14,15	0.53	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	1606	1	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
5	NAG	A	1603	1	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
5	NAG	D	1605	1	14,14,15	0.37	0	17,19,21	0.72	1 (5%)
5	NAG	B	1601	-	14,14,15	0.31	0	17,19,21	0.53	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
5	NAG	A	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1602	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1603	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1607	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1601	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1606	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1603	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1605	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1602	NAG	C1-O5-C5	4.07	117.64	112.19
5	C	1606	NAG	C1-O5-C5	3.07	116.29	112.19
5	A	1602	NAG	C1-O5-C5	2.98	116.17	112.19
5	B	1603	NAG	C1-O5-C5	2.97	116.17	112.19
5	A	1603	NAG	C1-O5-C5	2.81	115.96	112.19
5	D	1605	NAG	C1-O5-C5	2.68	115.78	112.19
5	D	1606	NAG	C1-O5-C5	2.52	115.56	112.19
5	B	1603	NAG	C1-C2-N2	2.32	114.09	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1111/1260 (88%)	-0.34	8 (0%) 84 73	22, 100, 190, 292	0
1	B	1120/1260 (88%)	-0.38	11 (0%) 79 67	23, 105, 185, 292	0
1	C	1113/1260 (88%)	-0.34	6 (0%) 87 77	56, 165, 300, 300	0
1	D	1123/1260 (89%)	-0.24	24 (2%) 63 54	29, 114, 279, 300	0
All	All	4467/5040 (88%)	-0.32	49 (1%) 78 66	22, 120, 282, 300	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	85	PHE	4.0
1	B	241	THR	3.9
1	C	28	SER	3.9
1	C	1399	LEU	3.7
1	C	1207	SER	3.6
1	A	1457	TRP	3.4
1	C	1206	ALA	3.3
1	D	1206	ALA	3.2
1	D	63	LEU	3.2
1	D	52	ALA	3.2
1	D	44	TYR	3.1
1	A	994	VAL	3.1
1	D	49	LEU	3.0
1	B	933	LEU	2.9
1	D	33	VAL	2.8
1	B	1327	ALA	2.8
1	D	1359	SER	2.7
1	D	912	PHE	2.7
1	A	993	VAL	2.7
1	D	1284	ILE	2.7
1	D	227	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	374	LEU	2.6
1	D	1436	LEU	2.5
1	D	1205	VAL	2.5
1	D	165	ASP	2.4
1	B	791	PHE	2.4
1	D	1014	ASP	2.4
1	A	1014	ASP	2.3
1	C	669	VAL	2.3
1	B	364	GLN	2.2
1	B	1326	PHE	2.2
1	D	1210	LEU	2.2
1	D	231	GLY	2.2
1	A	872	SER	2.2
1	D	1065	ASN	2.2
1	D	325	LEU	2.2
1	A	131	LEU	2.2
1	D	1399	LEU	2.2
1	C	1084	LYS	2.1
1	D	769	LEU	2.1
1	B	45	LEU	2.1
1	B	1233	TRP	2.1
1	D	1084	LYS	2.1
1	A	148	GLN	2.1
1	B	1324	TYR	2.1
1	A	234	VAL	2.1
1	B	370	LEU	2.1
1	B	1416	TRP	2.0
1	D	1374	ALA	2.0

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

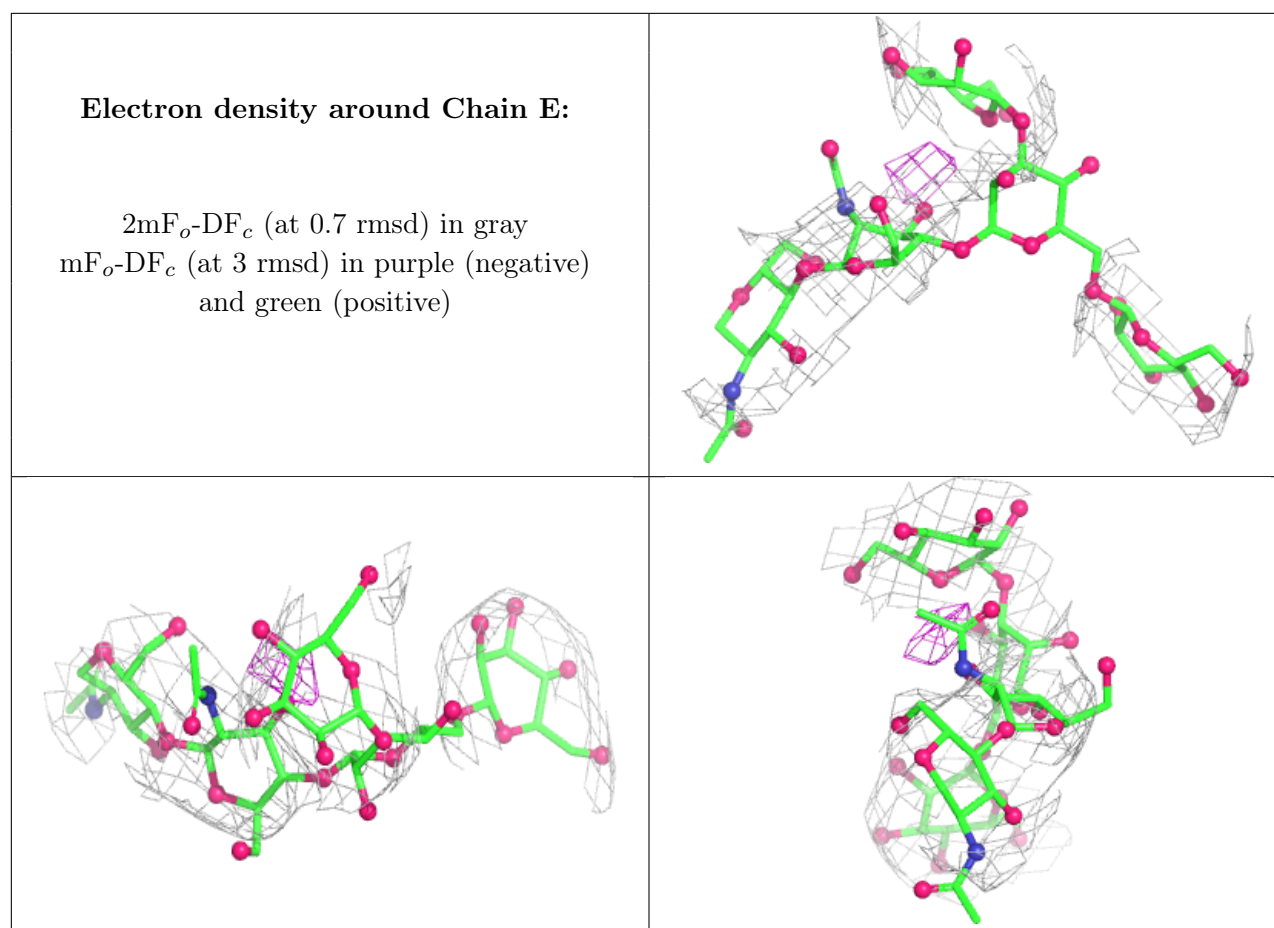
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

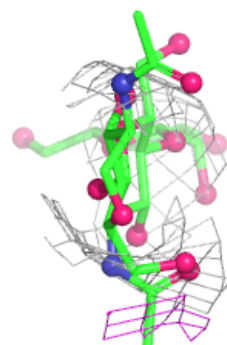
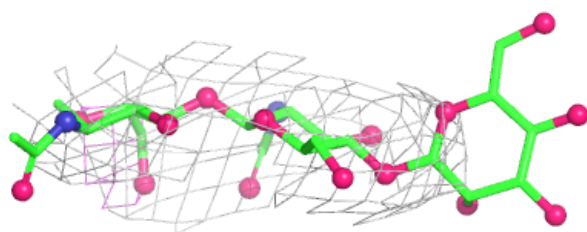
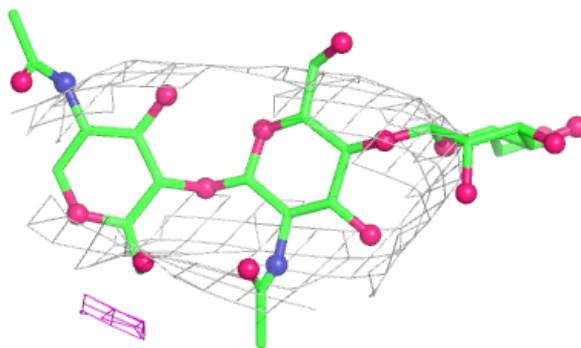
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	H	3	11/12	0.36	0.14	270,279,283,286	0
3	NAG	H	2	14/15	0.55	0.11	178,199,259,268	0
2	BMA	E	3	11/12	0.55	0.08	234,265,279,280	0
4	BMA	G	3	11/12	0.65	0.07	283,284,285,285	0
3	BMA	F	3	11/12	0.68	0.06	273,297,300,300	0
2	MAN	E	4	11/12	0.68	0.10	68,78,97,105	0
2	MAN	E	5	11/12	0.69	0.10	99,119,146,149	0
4	MAN	G	4	11/12	0.73	0.19	139,177,250,260	0
4	NAG	G	2	14/15	0.74	0.10	212,277,285,286	0
3	NAG	F	2	14/15	0.79	0.07	167,184,223,252	0
2	NAG	E	1	14/15	0.90	0.09	119,132,157,157	0
2	NAG	E	2	14/15	0.90	0.10	148,183,239,243	0
4	NAG	G	1	14/15	0.94	0.12	169,178,200,205	0
3	NAG	H	1	14/15	0.94	0.09	141,151,174,177	0
3	NAG	F	1	14/15	0.95	0.06	126,135,157,162	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.

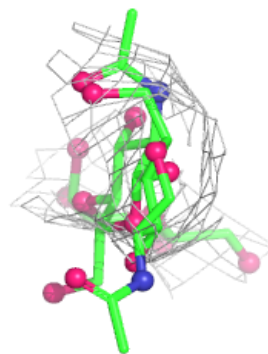
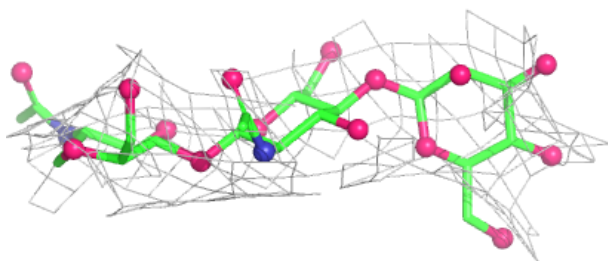
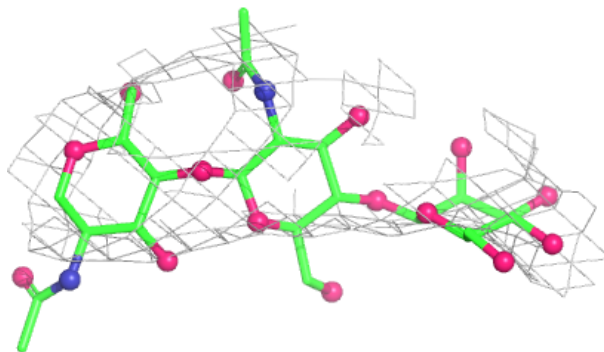


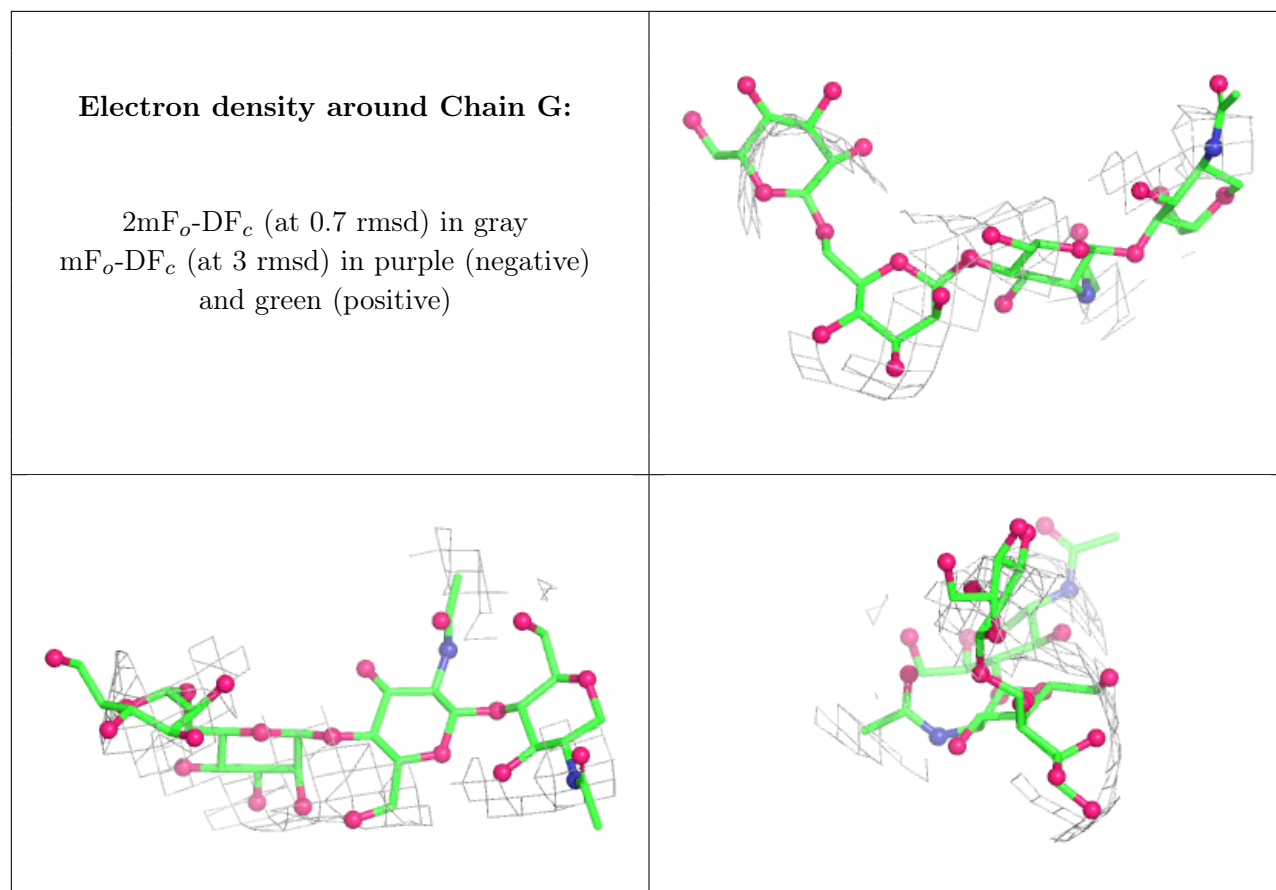
Electron density around Chain F:

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

**Electron density around Chain H:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	1601	14/15	0.45	0.22	148,153,161,162	0
5	NAG	C	1601	14/15	0.55	0.11	148,153,161,162	0
5	NAG	C	1606	14/15	0.57	0.06	292,292,293,293	0
5	NAG	D	1601	14/15	0.67	0.11	148,153,161,162	0
5	NAG	B	1603	14/15	0.68	0.09	189,255,283,283	0
5	NAG	A	1602	14/15	0.69	0.10	250,256,259,262	0
5	NAG	B	1601	14/15	0.69	0.11	148,153,161,162	0
5	NAG	C	1607	14/15	0.71	0.09	295,295,295,296	0
5	NAG	A	1603	14/15	0.71	0.10	199,247,278,280	0
5	NAG	D	1605	14/15	0.79	0.07	282,282,282,283	0
5	NAG	B	1602	14/15	0.82	0.09	250,257,261,262	0
6	CA	C	1608	1/1	0.85	0.14	234,234,234,234	1
5	NAG	D	1606	14/15	0.87	0.10	218,227,252,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	D	1607	1/1	0.97	0.11	191,191,191,191	1
6	CA	A	1604	1/1	0.98	0.04	152,152,152,152	1
6	CA	B	1604	1/1	1.00	0.03	142,142,142,142	1

6.5 Other polymers [i](#)

There are no such residues in this entry.