Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 06:51 AM EDT

PDB ID	:	2HPA
Title	:	STRUCTURAL ORIGINS OF L(+)-TARTRATE INHIBITION OF HUMAN PROSTATIC ACID PHOSPHATASE
Authors	:	Lacount, M.W.; Handy, G.; Lebioda, L.
Deposited on	:	1998-09-11
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

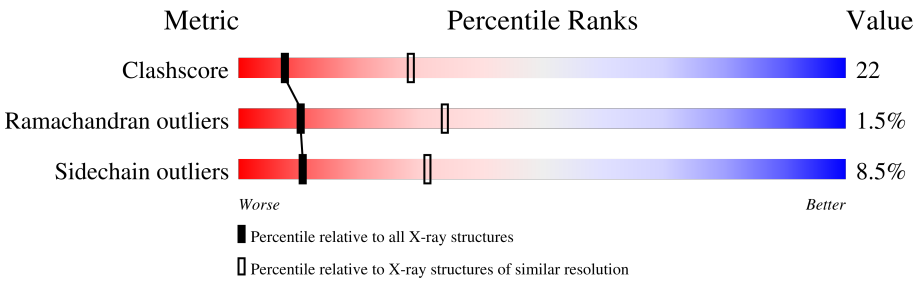
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	342	58% 35% 6%
1	B	342	55% 40% 5%
1	C	342	50% 44% 6%
1	D	342	51% 43% 5% •
2	E	3	33% 67%
3	F	2	100%
4	G	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1371	X	-	-	-
6	PT3	B	2345	-	-	X	-
6	PT3	D	4345	-	-	X	-

2 Entry composition (i)

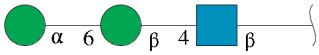
There are 7 unique types of molecules in this entry. The entry contains 11766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (ACID PHOSPHATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2801	1807	461	517	16	0	0	0
1	B	342	2801	1807	461	517	16	0	0	0
1	C	342	2801	1807	461	517	16	0	0	0
1	D	342	2801	1807	461	517	16	0	0	0

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



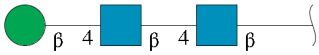
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	36	20	1	15	0	0	0

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

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

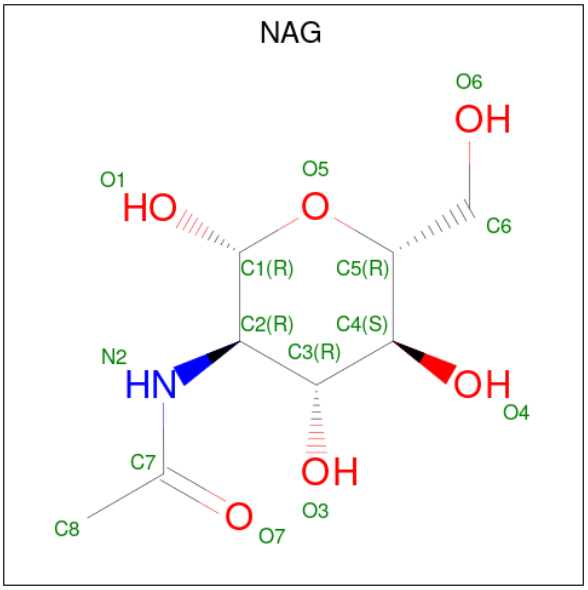
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

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



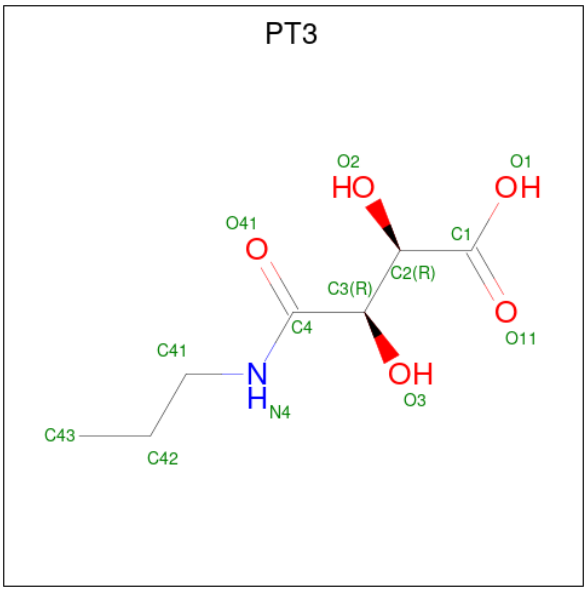
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	3	39	22	2	15	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is N-PROPYL-TARTRAMIC ACID (three-letter code: PT3) (formula: $C_7H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	13	7	1	5	0	0
			Total	C	N	O		
6	B	1	13	7	1	5	0	0
			Total	C	N	O		
6	D	1	13	7	1	5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	150	150	150	0	0
			Total	O		
7	B	84	84	84	0	0
			Total	O		
7	C	79	79	79	0	0
			Total	O		
7	D	37	37	37	0	0

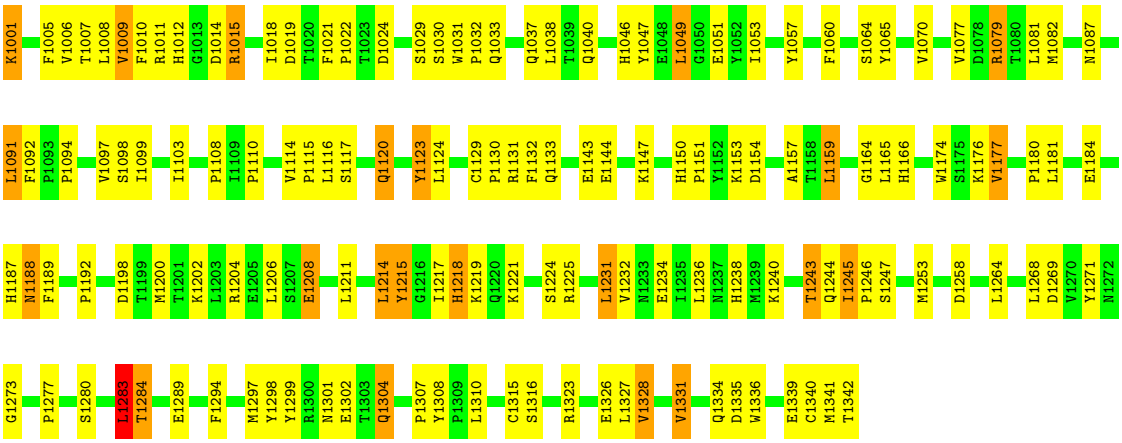
3 Residue-property plots (i)

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

Note EDS was not executed.

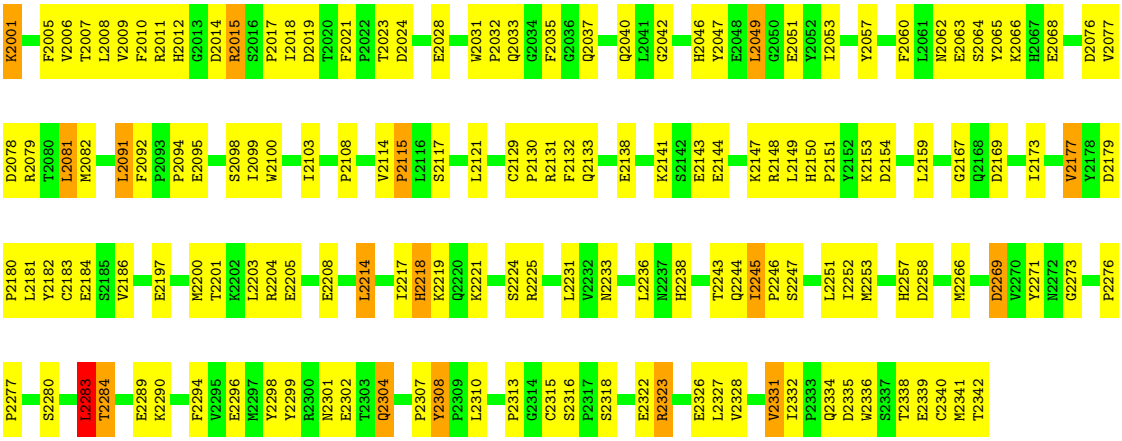
• Molecule 1: PROTEIN (ACID PHOSPHATASE)

Chain A: 58% 35% 6%



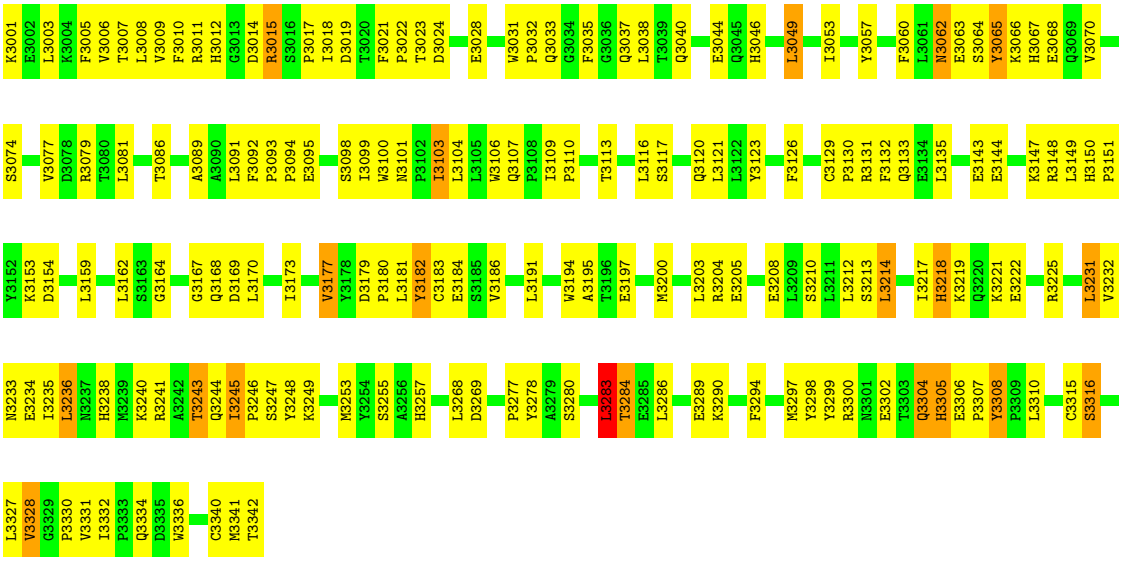
• Molecule 1: PROTEIN (ACID PHOSPHATASE)

Chain B: 55% 40% 5%



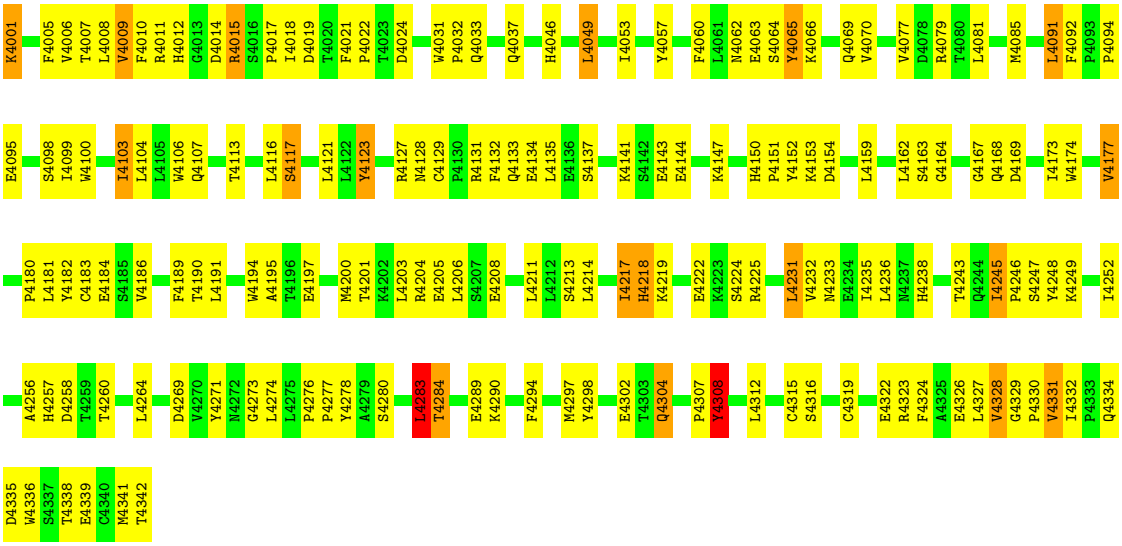
• Molecule 1: PROTEIN (ACID PHOSPHATASE)

Chain C: 50% 44% 6%



• Molecule 1: PROTEIN (ACID PHOSPHATASE)

Chain D:

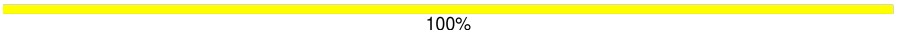


• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:



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

Chain G:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.86Å 202.68Å 71.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	88.3 (8.00-2.90)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.211 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11766	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

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, MAN, NAG, PT3

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	0.63	4/2883 (0.1%)	0.79	3/3914 (0.1%)
1	B	0.63	1/2883 (0.0%)	0.77	2/3914 (0.1%)
1	C	0.59	2/2883 (0.1%)	0.78	1/3914 (0.0%)
1	D	0.64	2/2883 (0.1%)	0.79	3/3914 (0.1%)
All	All	0.62	9/11532 (0.1%)	0.78	9/15656 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4308	TYR	CB-CG	-9.05	1.38	1.51
1	D	4308	TYR	CD2-CE2	-7.59	1.27	1.39
1	B	2184	GLU	CG-CD	-7.06	1.41	1.51
1	A	1208	GLU	CD-OE2	6.99	1.33	1.25
1	A	1208	GLU	CG-CD	-5.81	1.43	1.51
1	C	3062	ASN	CG-ND2	5.27	1.46	1.32
1	C	3308	TYR	CB-CG	-5.27	1.43	1.51
1	A	1188	ASN	CB-CG	5.24	1.63	1.51
1	A	1308	TYR	CB-CG	-5.01	1.44	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3283	LEU	CA-CB-CG	8.35	134.51	115.30
1	A	1208	GLU	OE1-CD-OE2	7.40	132.18	123.30
1	B	2283	LEU	CA-CB-CG	6.76	130.86	115.30
1	D	4283	LEU	CA-CB-CG	6.65	130.59	115.30
1	D	4308	TYR	N-CA-CB	-6.56	98.79	110.60
1	D	4308	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	1283	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	2184	GLU	CG-CD-OE1	-5.24	107.82	118.30
1	A	1079	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1215	TYR	Sidechain
1	B	2308	TYR	Sidechain
1	C	3182	TYR	Sidechain
1	D	4065	TYR	Sidechain
1	D	4308	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2801	0	2746	120	0
1	B	2801	0	2747	121	0
1	C	2801	0	2745	152	0
1	D	2801	0	2747	124	0
2	E	36	0	31	3	0
3	F	28	0	25	0	0
4	G	39	0	34	6	0
5	A	14	0	13	4	0
5	B	14	0	13	0	0
5	C	42	0	39	2	0
6	A	13	0	12	2	0
6	B	13	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	13	0	12	6	0
7	A	150	0	0	11	0
7	B	84	0	0	4	0
7	C	79	0	0	7	0
7	D	37	0	0	0	0
All	All	11766	0	11176	498	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 22.

All (498) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:HIS:HD2	5:A:1371:NAG:H83	1.23	1.01
1:A:1189:PHE:CE1	1:C:3245:ILE:HG22	1.99	0.97
1:D:4033:GLN:HB3	1:D:4037:GLN:HG2	1.49	0.92
1:C:3305:HIS:CE1	1:C:3306:GLU:HG2	2.08	0.88
1:A:1187:HIS:CD2	5:A:1371:NAG:H83	2.10	0.87
1:C:3033:GLN:HB3	1:C:3037:GLN:HG2	1.56	0.87
1:B:2225:ARG:HH22	1:B:2334:GLN:HG2	1.41	0.84
1:B:2182:TYR:O	1:B:2186:VAL:HG23	1.79	0.83
1:C:3218:HIS:NE2	1:C:3219:LYS:HD2	1.95	0.82
1:D:4225:ARG:HH22	1:D:4334:GLN:HG2	1.46	0.81
1:B:2091:LEU:HD13	1:B:2092:PHE:CE2	2.16	0.80
1:A:1245:ILE:HD12	1:A:1246:PRO:O	1.81	0.79
1:D:4091:LEU:HD13	1:D:4092:PHE:CE2	2.18	0.78
1:A:1225:ARG:HH22	1:A:1334:GLN:HG2	1.48	0.78
1:B:2094:PRO:HB2	1:B:2099:ILE:HG12	1.65	0.77
1:A:1192:PRO:HD3	7:A:5371:HOH:O	1.85	0.77
1:C:3094:PRO:HA	1:C:3098:SER:OG	1.84	0.77
1:B:2018:ILE:HG12	6:B:2345:PT3:H421	1.67	0.76
1:A:1189:PHE:HE1	1:C:3245:ILE:HG22	1.47	0.76
1:C:3277:PRO:HG2	1:C:3280:SER:HB3	1.67	0.74
1:A:1030:SER:HB3	1:C:3245:ILE:HB	1.68	0.74
1:A:1079:ARG:NH1	6:A:1345:PT3:O3	2.20	0.73
1:C:3113:THR:HG22	1:D:4113:THR:HG22	1.70	0.73
1:A:1225:ARG:NH2	1:A:1334:GLN:HG2	2.04	0.73
1:B:2033:GLN:HB3	1:B:2037:GLN:HG2	1.70	0.73
1:B:2200:MET:HG3	7:B:5397:HOH:O	1.86	0.73
1:C:3116:LEU:HD13	1:C:3123:TYR:CE2	2.23	0.73
1:D:4245:ILE:HD12	1:D:4246:PRO:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:PHE:HA	1:C:3244:GLN:NE2	2.04	0.72
1:B:2129:CYS:HB2	1:B:2336:TRP:CZ2	2.25	0.71
1:A:1129:CYS:HB2	1:A:1336:TRP:CZ2	2.26	0.71
1:A:1094:PRO:HB2	1:A:1099:ILE:HG12	1.72	0.71
1:B:2225:ARG:NH2	1:B:2334:GLN:HG2	2.05	0.71
1:A:1030:SER:OG	1:C:3245:ILE:HD13	1.91	0.70
1:B:2277:PRO:HG2	1:B:2280:SER:HB3	1.73	0.70
1:C:3225:ARG:HH22	1:C:3334:GLN:HG2	1.54	0.70
1:B:2018:ILE:HD12	1:B:2019:ASP:HB2	1.71	0.70
1:C:3104:LEU:HD11	1:D:4106:TRP:HB2	1.72	0.69
1:D:4131:ARG:HD3	1:D:4342:THR:HG21	1.73	0.69
1:C:3208:GLU:HB2	7:C:5099:HOH:O	1.92	0.69
7:A:5418:HOH:O	1:B:2033:GLN:HG3	1.92	0.69
7:A:5291:HOH:O	2:E:2:BMA:O2	2.08	0.69
1:B:2302:GLU:HB3	1:B:2304:GLN:OE1	1.91	0.69
1:A:1021:PHE:CZ	1:A:1024:ASP:HB2	2.27	0.69
1:A:1123:TYR:HB3	7:A:5064:HOH:O	1.93	0.69
1:D:4302:GLU:HB3	1:D:4304:GLN:OE1	1.93	0.69
1:D:4008:LEU:HD22	1:D:4283:LEU:HD13	1.74	0.69
1:B:2299:TYR:HB2	1:B:2310:LEU:HD11	1.73	0.68
1:D:4150:HIS:HB3	1:D:4151:PRO:HD3	1.74	0.68
1:D:4225:ARG:NH2	1:D:4334:GLN:HG2	2.08	0.68
1:C:3290:LYS:HB2	1:C:3290:LYS:NZ	2.08	0.68
1:A:1008:LEU:HD22	1:A:1283:LEU:HD13	1.76	0.68
4:G:1:NAG:H62	4:G:2:NAG:H82	1.77	0.67
1:C:3007:THR:HB	1:C:3284:THR:HG23	1.77	0.67
1:C:3299:TYR:HB2	1:C:3310:LEU:HD11	1.77	0.67
1:C:3302:GLU:HB3	1:C:3304:GLN:OE1	1.95	0.67
1:D:4290:LYS:HB2	1:D:4290:LYS:NZ	2.09	0.67
1:C:3245:ILE:HD12	1:C:3246:PRO:O	1.96	0.66
1:A:1131:ARG:HD3	1:A:1342:THR:HG21	1.77	0.66
1:D:4079:ARG:NH1	6:D:4345:PT3:O3	2.28	0.66
1:B:2131:ARG:HD3	1:B:2342:THR:HG21	1.77	0.65
1:B:2062:ASN:O	1:B:2063:GLU:HG3	1.96	0.65
1:C:3006:VAL:HG12	1:C:3060:PHE:HE2	1.62	0.65
1:B:2006:VAL:HG21	1:B:2057:TYR:OH	1.97	0.65
1:A:1130:PRO:HD2	1:A:1340:CYS:HB3	1.78	0.65
1:B:2028:GLU:HA	1:B:2035:PHE:CE1	2.32	0.64
1:C:3305:HIS:ND1	1:C:3306:GLU:N	2.46	0.64
1:D:4129:CYS:HB2	1:D:4336:TRP:CZ2	2.32	0.64
1:D:4257:HIS:HB3	6:D:4345:PT3:O2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2245:ILE:HD12	1:B:2246:PRO:O	1.98	0.64
1:C:3150:HIS:HA	1:C:3153:LYS:HD3	1.79	0.64
1:A:1015:ARG:NH1	6:A:1345:PT3:O1	2.30	0.64
1:A:1132:PHE:HZ	1:A:1214:LEU:HD23	1.63	0.64
1:D:4094:PRO:HA	1:D:4098:SER:OG	1.98	0.64
1:D:4341:MET:O	1:D:4342:THR:HB	1.98	0.64
1:D:4094:PRO:HB2	1:D:4099:ILE:HG12	1.80	0.63
1:B:2150:HIS:HA	1:B:2153:LYS:HD3	1.80	0.63
1:D:4277:PRO:HG2	1:D:4280:SER:HB3	1.80	0.63
1:C:3106:TRP:HB2	1:D:4104:LEU:HD11	1.80	0.63
1:C:3010:PHE:CD1	1:C:3046:HIS:HE1	2.17	0.63
1:D:4007:THR:HB	1:D:4284:THR:HG23	1.80	0.63
1:A:1341:MET:O	1:A:1342:THR:HB	1.99	0.63
1:B:2204:ARG:O	1:B:2208:GLU:HG3	1.98	0.63
1:A:1181:LEU:HD13	1:A:1200:MET:HE3	1.81	0.62
1:C:3300:ARG:NE	7:C:5443:HOH:O	2.31	0.62
1:C:3094:PRO:HB2	1:C:3099:ILE:HG12	1.81	0.62
1:A:1204:ARG:NH1	7:A:5375:HOH:O	2.28	0.61
1:D:4173:ILE:O	1:D:4177:VAL:HG13	2.01	0.61
1:A:1150:HIS:HA	1:A:1153:LYS:HD3	1.81	0.61
1:A:1143:GLU:HG3	1:A:1144:GLU:N	2.14	0.61
1:B:2201:THR:O	1:B:2205:GLU:HG3	2.00	0.61
1:A:1006:VAL:HG12	1:A:1060:PHE:HE2	1.66	0.61
1:D:4057:TYR:HB3	1:D:4060:PHE:HB3	1.81	0.61
1:D:4335:ASP:O	1:D:4339:GLU:HG3	2.01	0.61
1:C:3038:LEU:N	7:C:5411:HOH:O	2.28	0.61
1:B:2079:ARG:NH1	6:B:2345:PT3:O3	2.34	0.60
1:B:2049:LEU:HD22	1:B:2049:LEU:O	2.01	0.60
1:C:3021:PHE:CZ	1:C:3024:ASP:HB2	2.36	0.60
1:C:3033:GLN:CB	1:C:3037:GLN:HG2	2.29	0.60
1:A:1315:CYS:HB2	1:A:1327:LEU:CD1	2.31	0.60
1:B:2335:ASP:O	1:B:2339:GLU:HG3	2.01	0.60
1:C:3063:GLU:HG3	5:C:3361:NAG:H82	1.83	0.60
1:D:4308:TYR:CE2	4:G:1:NAG:O6	2.53	0.60
1:D:4245:ILE:HG13	1:D:4245:ILE:O	2.02	0.60
1:C:3212:LEU:HD11	7:C:5334:HOH:O	2.02	0.59
1:A:1302:GLU:HB3	1:A:1304:GLN:OE1	2.01	0.59
1:D:4233:ASN:HB2	1:D:4332:ILE:HG23	1.84	0.59
1:A:1012:HIS:CE1	1:A:1015:ARG:HD3	2.36	0.59
1:B:2144:GLU:O	1:B:2148:ARG:HG3	2.03	0.59
1:B:2173:ILE:O	1:B:2177:VAL:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3225:ARG:NH2	1:C:3334:GLN:HG2	2.16	0.59
1:C:3182:TYR:O	1:C:3186:VAL:HG23	2.01	0.59
1:D:4150:HIS:HA	1:D:4153:LYS:HD3	1.85	0.59
1:B:2010:PHE:CE2	1:B:2253:MET:HE3	2.38	0.59
1:A:1289:GLU:HB3	1:A:1294:PHE:HE2	1.68	0.59
1:B:2245:ILE:O	1:B:2245:ILE:HG13	2.02	0.59
1:A:1007:THR:HB	1:A:1284:THR:HG23	1.85	0.58
1:A:1218:HIS:NE2	1:A:1219:LYS:HD2	2.18	0.58
1:C:3062:ASN:O	1:C:3063:GLU:HG3	2.03	0.58
1:B:2018:ILE:HG13	7:B:5023:HOH:O	2.04	0.58
1:B:2290:LYS:HB2	1:B:2290:LYS:NZ	2.19	0.58
1:C:3290:LYS:HB2	1:C:3290:LYS:HZ2	1.68	0.58
1:A:1180:PRO:O	1:A:1184:GLU:HG3	2.04	0.58
1:B:2218:HIS:NE2	1:B:2219:LYS:HD2	2.18	0.58
1:C:3008:LEU:HD22	1:C:3283:LEU:HD13	1.85	0.57
1:C:3181:LEU:HD13	1:C:3200:MET:HE3	1.84	0.57
1:C:3104:LEU:HD12	1:D:4104:LEU:HD12	1.86	0.57
1:C:3186:VAL:O	5:C:3371:NAG:H82	2.03	0.57
1:B:2094:PRO:CB	1:B:2099:ILE:HG12	2.34	0.57
1:C:3173:ILE:O	1:C:3177:VAL:HG13	2.05	0.57
1:D:4174:TRP:CH2	1:D:4211:LEU:HD13	2.40	0.57
1:A:1094:PRO:HA	1:A:1098:SER:OG	2.05	0.56
1:B:2130:PRO:HD2	1:B:2340:CYS:HB3	1.86	0.56
1:C:3218:HIS:HE2	1:C:3219:LYS:HD2	1.68	0.56
1:D:4010:PHE:CD1	1:D:4046:HIS:HE1	2.24	0.56
1:A:1335:ASP:O	1:A:1339:GLU:HG3	2.06	0.56
1:D:4298:TYR:HB3	1:D:4307:PRO:HB2	1.86	0.56
1:A:1299:TYR:HB2	1:A:1310:LEU:HD11	1.86	0.55
1:B:2077:VAL:O	1:B:2081:LEU:HD22	2.06	0.55
1:B:2296:GLU:HG2	1:B:2318:SER:HA	1.87	0.55
1:B:2179:ASP:HB3	1:B:2180:PRO:HD3	1.87	0.55
1:D:4137:SER:O	1:D:4141:LYS:HG3	2.07	0.55
1:A:1150:HIS:HB3	1:A:1151:PRO:HD3	1.89	0.55
1:C:3181:LEU:HD13	1:C:3200:MET:CE	2.36	0.55
1:D:4204:ARG:O	1:D:4208:GLU:HG3	2.07	0.55
1:A:1010:PHE:CD1	1:A:1046:HIS:HE1	2.25	0.55
1:B:2010:PHE:CD1	1:B:2046:HIS:HE1	2.25	0.55
1:C:3315:CYS:HB2	1:C:3327:LEU:CD1	2.37	0.55
1:B:2289:GLU:HB3	1:B:2294:PHE:HE1	1.71	0.55
1:A:1091:LEU:HD13	1:A:1092:PHE:CE2	2.41	0.55
1:B:2181:LEU:HD13	1:B:2200:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4201:THR:O	1:D:4205:GLU:HG3	2.07	0.54
1:C:3005:PHE:CZ	1:C:3238:HIS:HB3	2.43	0.54
1:C:3018:ILE:HD12	1:C:3019:ASP:HB2	1.88	0.54
1:C:3305:HIS:ND1	1:C:3306:GLU:HG2	2.22	0.54
1:C:3023:THR:HG22	1:C:3023:THR:O	2.07	0.54
1:B:2177:VAL:C	1:B:2180:PRO:HD2	2.28	0.54
1:C:3101:ASN:OD1	1:C:3103:ILE:HD12	2.07	0.54
1:D:4200:MET:CE	1:D:4203:LEU:HD12	2.37	0.54
1:B:2150:HIS:HB3	1:B:2151:PRO:HD3	1.90	0.54
1:C:3341:MET:O	1:C:3342:THR:HB	2.07	0.54
1:A:1011:ARG:NE	1:A:1258:ASP:HB3	2.23	0.54
1:C:3012:HIS:NE2	1:C:3079:ARG:HD2	2.22	0.54
1:A:1012:HIS:CE1	1:A:1015:ARG:HG2	2.43	0.53
1:C:3131:ARG:HD3	1:C:3342:THR:HG21	1.89	0.53
1:D:4181:LEU:HD13	1:D:4200:MET:HE3	1.90	0.53
1:B:2006:VAL:HG12	1:B:2060:PHE:HE2	1.74	0.53
1:A:1204:ARG:O	1:A:1208:GLU:HG3	2.08	0.53
1:B:2066:LYS:HB3	1:B:2068:GLU:OE2	2.08	0.53
1:C:3236:LEU:O	1:C:3240:LYS:HG3	2.09	0.53
1:C:3298:TYR:HB3	1:C:3307:PRO:HB2	1.91	0.53
1:A:1012:HIS:HE1	1:A:1015:ARG:HD3	1.73	0.53
2:E:1:NAG:H62	2:E:2:BMA:H2	1.89	0.53
1:A:1012:HIS:HE1	1:A:1015:ARG:HG2	1.74	0.53
1:A:1298:TYR:HB3	1:A:1307:PRO:HB2	1.90	0.53
1:D:4095:GLU:H	1:D:4098:SER:HB3	1.73	0.53
1:B:2323:ARG:HA	1:B:2326:GLU:HG2	1.91	0.52
1:D:4079:ARG:HH12	6:D:4345:PT3:C4	2.22	0.52
1:A:1164:GLY:HA2	1:D:4117:SER:HB3	1.90	0.52
1:B:2148:ARG:HA	7:B:5049:HOH:O	2.09	0.52
1:A:1014:ASP:O	1:A:1038:LEU:HD12	2.10	0.52
1:A:1132:PHE:HZ	1:A:1214:LEU:CD2	2.23	0.52
1:B:2021:PHE:CZ	1:B:2024:ASP:HB2	2.45	0.52
1:B:2001:LYS:NZ	1:B:2001:LYS:HB3	2.24	0.52
1:B:2301:ASN:O	1:B:2302:GLU:HG3	2.10	0.52
1:A:1097:VAL:O	1:B:2040:GLN:NE2	2.41	0.52
1:C:3067:HIS:O	1:C:3249:LYS:NZ	2.43	0.52
1:D:4015:ARG:NH1	6:D:4345:PT3:O1	2.43	0.52
1:C:3095:GLU:O	1:C:3098:SER:HB3	2.10	0.52
1:D:4022:PRO:HG2	1:D:4164:GLY:HA3	1.92	0.52
1:C:3010:PHE:CD1	1:C:3046:HIS:CE1	2.98	0.52
1:C:3233:ASN:HB2	1:C:3332:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1:NAG:H62	4:G:2:NAG:C8	2.40	0.52
1:A:1006:VAL:HG21	1:A:1057:TYR:OH	2.10	0.52
1:A:1022:PRO:HG2	1:A:1164:GLY:HA3	1.92	0.52
1:A:1166:HIS:ND1	1:D:4128:ASN:HB3	2.25	0.52
1:D:4271:TYR:CE2	1:D:4273:GLY:HA2	2.44	0.51
1:A:1323:ARG:HA	1:A:1326:GLU:HG2	1.91	0.51
1:C:3130:PRO:HD2	1:C:3340:CYS:HB3	1.92	0.51
1:A:1033:GLN:HB3	1:A:1037:GLN:HG2	1.92	0.51
1:C:3010:PHE:CE2	1:C:3253:MET:HE3	2.46	0.51
1:C:3241:ARG:HD2	1:C:3248:TYR:OH	2.11	0.51
1:D:4008:LEU:CD2	1:D:4283:LEU:HD13	2.40	0.51
1:D:4001:LYS:HB3	1:D:4001:LYS:NZ	2.26	0.51
1:A:1240:LYS:HB3	7:A:5053:HOH:O	2.10	0.51
1:B:2008:LEU:HD22	1:B:2283:LEU:HD13	1.92	0.51
1:C:3179:ASP:HB3	1:C:3180:PRO:HD3	1.92	0.51
1:A:1077:VAL:HG23	1:A:1116:LEU:HD21	1.93	0.51
1:C:3014:ASP:HA	1:C:3278:TYR:CD1	2.46	0.50
1:A:1010:PHE:CE2	1:A:1253:MET:HE3	2.46	0.50
1:A:1245:ILE:O	1:A:1245:ILE:HG13	2.11	0.50
1:B:2132:PHE:HZ	1:B:2214:LEU:HD23	1.76	0.50
1:B:2012:HIS:CE1	1:B:2015:ARG:HG2	2.45	0.50
1:C:3074:SER:HB2	1:C:3255:SER:HB3	1.94	0.50
1:C:3150:HIS:HB3	1:C:3151:PRO:HD3	1.92	0.50
1:A:1159:LEU:HD11	1:A:1177:VAL:HG21	1.94	0.50
1:A:1005:PHE:CZ	1:A:1238:HIS:HB3	2.47	0.50
1:A:1177:VAL:C	1:A:1180:PRO:HD2	2.31	0.50
1:B:2095:GLU:O	1:B:2098:SER:HB3	2.11	0.50
1:A:1029:SER:HB2	1:C:3247:SER:CB	2.42	0.50
1:A:1047:TYR:O	1:A:1051:GLU:HG3	2.12	0.50
1:B:2271:TYR:CE2	1:B:2273:GLY:HA2	2.46	0.50
1:B:2290:LYS:HB2	1:B:2290:LYS:HZ2	1.77	0.50
1:D:4322:GLU:CD	1:D:4322:GLU:H	2.15	0.50
1:C:3086:THR:O	1:C:3089:ALA:HB3	2.12	0.50
1:C:3200:MET:CE	1:C:3203:LEU:HD12	2.42	0.50
1:D:4289:GLU:HB3	1:D:4294:PHE:HE1	1.78	0.49
1:A:1077:VAL:HG11	1:A:1079:ARG:CZ	2.42	0.49
1:B:2010:PHE:HE2	1:B:2253:MET:HE3	1.75	0.49
1:B:2269:ASP:HB3	1:B:2313:PRO:HG3	1.94	0.49
1:D:4005:PHE:CZ	1:D:4238:HIS:HB3	2.46	0.49
1:D:4283:LEU:O	1:D:4297:MET:HA	2.12	0.49
1:C:3149:LEU:HG	1:C:3153:LYS:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4116:LEU:HD22	1:D:4123:TYR:CD2	2.47	0.49
1:A:1021:PHE:CE1	1:A:1024:ASP:HB2	2.47	0.49
1:B:2028:GLU:HA	1:B:2035:PHE:CZ	2.46	0.49
1:B:2266:MET:SD	1:B:2271:TYR:CD2	3.05	0.49
1:C:3212:LEU:CD1	7:C:5334:HOH:O	2.60	0.49
1:D:4095:GLU:N	1:D:4098:SER:HB3	2.28	0.49
1:A:1129:CYS:O	1:A:1133:GLN:HG2	2.12	0.49
1:B:2289:GLU:HG3	1:B:2290:LYS:HE3	1.95	0.49
1:B:2315:CYS:HB2	1:B:2327:LEU:CD1	2.42	0.49
1:C:3070:VAL:HG21	1:C:3092:PHE:CZ	2.47	0.49
1:D:4012:HIS:CE1	1:D:4015:ARG:HD3	2.48	0.49
1:D:4290:LYS:HB2	1:D:4290:LYS:HZ2	1.74	0.49
1:C:3144:GLU:O	1:C:3148:ARG:HG3	2.13	0.49
1:D:4177:VAL:C	1:D:4180:PRO:HD2	2.33	0.49
1:B:2289:GLU:HB3	1:B:2294:PHE:CE1	2.48	0.49
1:C:3103:ILE:HD12	1:C:3103:ILE:H	1.78	0.48
1:C:3240:LYS:O	1:C:3243:THR:HB	2.13	0.48
1:D:4289:GLU:HB3	1:D:4294:PHE:CE1	2.48	0.48
1:A:1268:LEU:HD13	1:A:1297:MET:SD	2.54	0.48
1:C:3218:HIS:CE1	1:C:3219:LYS:HD2	2.47	0.48
1:D:4274:LEU:HD12	4:G:1:NAG:H4	1.95	0.48
1:A:1157:ALA:HA	7:A:5082:HOH:O	2.14	0.48
1:B:2019:ASP:O	1:B:2180:PRO:HG3	2.13	0.48
1:B:2200:MET:CE	1:B:2203:LEU:HD12	2.43	0.48
1:B:2233:ASN:HB2	1:B:2332:ILE:HG23	1.95	0.48
1:B:2129:CYS:O	1:B:2133:GLN:HG2	2.14	0.48
1:B:2224:SER:HB3	1:B:2331:VAL:HG22	1.95	0.48
1:C:3017:PRO:HG3	1:C:3183:CYS:HB2	1.95	0.48
1:D:4011:ARG:HD2	1:D:4258:ASP:HB3	1.95	0.48
1:D:4135:LEU:HD11	1:D:4222:GLU:HG2	1.95	0.48
1:C:3021:PHE:CE2	1:C:3024:ASP:HB2	2.48	0.48
1:C:3094:PRO:HG2	1:C:3106:TRP:N	2.29	0.48
1:B:2143:GLU:HG3	1:B:2144:GLU:N	2.29	0.48
1:C:3167:GLY:C	1:C:3169:ASP:H	2.17	0.48
1:C:3231:LEU:O	1:C:3234:GLU:HB3	2.14	0.48
1:D:4232:VAL:HG11	1:D:4328:VAL:HG22	1.95	0.48
1:A:1231:LEU:HD13	1:A:1264:LEU:HD22	1.96	0.48
1:C:3135:LEU:CD2	1:C:3219:LYS:HD3	2.43	0.48
1:A:1166:HIS:HB2	1:D:4127:ARG:HB2	1.96	0.47
1:B:2138:GLU:O	1:B:2141:LYS:N	2.47	0.47
1:C:3315:CYS:SG	1:C:3316:SER:N	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4019:ASP:O	1:D:4180:PRO:HG3	2.14	0.47
1:C:3129:CYS:HB2	1:C:3336:TRP:CZ2	2.49	0.47
1:C:3040:GLN:O	1:C:3044:GLU:HG3	2.14	0.47
1:B:2246:PRO:O	1:B:2247:SER:HB2	2.14	0.47
1:B:2298:TYR:HB3	1:B:2307:PRO:HB2	1.95	0.47
1:C:3177:VAL:C	1:C:3180:PRO:HD2	2.35	0.47
1:B:2076:ASP:HB2	1:B:2114:VAL:O	2.14	0.47
1:C:3053:ILE:HG23	1:C:3057:TYR:CE2	2.50	0.47
1:C:3162:LEU:HD13	1:C:3194:TRP:HB2	1.95	0.47
1:D:4010:PHE:CD1	1:D:4046:HIS:CE1	3.02	0.47
1:A:1006:VAL:HG12	1:A:1060:PHE:CE2	2.48	0.47
1:B:2049:LEU:O	1:B:2053:ILE:HG12	2.15	0.47
1:B:2079:ARG:HH12	6:B:2345:PT3:C4	2.28	0.47
1:C:3014:ASP:HA	1:C:3278:TYR:CE1	2.50	0.47
1:D:4132:PHE:HD2	1:D:4133:GLN:NE2	2.12	0.47
1:C:3120:GLN:HA	1:C:3126:PHE:CE1	2.50	0.47
1:A:1181:LEU:HD13	1:A:1200:MET:CE	2.43	0.47
1:A:1198:ASP:O	1:A:1202:LYS:HG2	2.15	0.47
1:C:3245:ILE:HG13	1:C:3248:TYR:HB2	1.96	0.47
1:B:2012:HIS:HE1	1:B:2015:ARG:HG2	1.80	0.47
1:B:2114:VAL:HG13	1:B:2115:PRO:HD2	1.96	0.47
1:B:2218:HIS:HE2	1:B:2219:LYS:HD2	1.80	0.47
1:D:4246:PRO:O	1:D:4247:SER:HB2	2.14	0.46
1:A:1038:LEU:CB	7:A:5252:HOH:O	2.63	0.46
1:A:1240:LYS:HE2	7:A:5053:HOH:O	2.16	0.46
1:B:2006:VAL:HG12	1:B:2060:PHE:CE2	2.50	0.46
1:C:3049:LEU:O	1:C:3053:ILE:HG12	2.15	0.46
1:B:2010:PHE:CD1	1:B:2046:HIS:CE1	3.03	0.46
1:B:2114:VAL:CG1	1:B:2115:PRO:HD2	2.45	0.46
1:C:3028:GLU:HA	1:C:3035:PHE:CE1	2.51	0.46
1:C:3232:VAL:HG11	1:C:3328:VAL:CG2	2.45	0.46
1:A:1001:LYS:NZ	1:A:1001:LYS:HB3	2.31	0.46
1:A:1053:ILE:HG23	1:A:1057:TYR:CE2	2.50	0.46
1:C:3012:HIS:CE1	1:C:3015:ARG:HD3	2.51	0.46
1:C:3049:LEU:O	1:C:3049:LEU:HD22	2.14	0.46
1:D:4233:ASN:HB2	1:D:4332:ILE:CG2	2.44	0.46
1:A:1030:SER:HB3	1:C:3245:ILE:CB	2.42	0.46
1:A:1120:GLN:O	1:A:1120:GLN:HG3	2.15	0.46
1:D:4005:PHE:HD1	1:D:4249:LYS:O	1.98	0.46
1:A:1108:PRO:O	1:B:2082:MET:HE3	2.16	0.46
1:A:1184:GLU:HA	1:A:1189:PHE:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3095:GLU:N	1:C:3098:SER:HB3	2.30	0.46
1:D:4022:PRO:HG2	1:D:4163:SER:O	2.16	0.46
1:A:1031:TRP:HA	1:A:1032:PRO:HD2	1.79	0.45
1:A:1189:PHE:HA	1:C:3244:GLN:HE21	1.79	0.45
1:C:3066:LYS:HB3	1:C:3068:GLU:OE2	2.16	0.45
1:C:3213:SER:HB3	1:C:3217:ILE:HD11	1.98	0.45
1:B:2094:PRO:HA	1:B:2098:SER:OG	2.15	0.45
1:B:2221:LYS:HD3	1:B:2331:VAL:HG23	1.98	0.45
1:D:4152:TYR:CG	1:D:4206:LEU:HD21	2.51	0.45
1:D:4232:VAL:HG11	1:D:4328:VAL:CG2	2.46	0.45
1:A:1030:SER:CB	1:C:3245:ILE:HD13	2.46	0.45
1:A:1341:MET:O	1:A:1342:THR:CB	2.63	0.45
1:C:3132:PHE:HD2	1:C:3133:GLN:NE2	2.14	0.45
1:C:3205:GLU:HA	7:C:5099:HOH:O	2.16	0.45
1:C:3268:LEU:HD13	1:C:3297:MET:SD	2.56	0.45
1:D:4217:ILE:HD13	1:D:4217:ILE:HG21	1.68	0.45
1:B:2015:ARG:NH1	6:B:2345:PT3:O1	2.49	0.45
1:B:2200:MET:HE2	1:B:2200:MET:HA	1.98	0.45
1:A:1143:GLU:HG3	1:A:1144:GLU:H	1.82	0.45
1:C:3246:PRO:O	1:C:3247:SER:HB2	2.16	0.45
1:D:4007:THR:HG21	1:D:4235:ILE:HG12	1.99	0.45
1:D:4162:LEU:HD13	1:D:4194:TRP:CB	2.47	0.45
1:D:4342:THR:HG23	1:D:4342:THR:O	2.16	0.45
1:A:1008:LEU:CD2	1:A:1283:LEU:HD13	2.46	0.45
1:B:2012:HIS:CE1	1:B:2015:ARG:HD3	2.52	0.45
1:A:1208:GLU:CD	7:A:5375:HOH:O	2.54	0.45
1:C:3110:PRO:HA	1:D:4085:MET:HE1	1.99	0.45
1:D:4308:TYR:CD2	4:G:1:NAG:O6	2.70	0.45
1:D:4315:CYS:HB2	1:D:4327:LEU:CD1	2.46	0.45
1:B:2014:ASP:H	1:B:2042:GLY:HA2	1.81	0.45
1:D:4095:GLU:O	1:D:4098:SER:HB3	2.17	0.45
1:D:4200:MET:HE2	1:D:4203:LEU:HD12	1.98	0.45
1:A:1271:TYR:CE2	1:A:1273:GLY:HA2	2.52	0.44
1:A:1283:LEU:O	1:A:1297:MET:HA	2.17	0.44
1:C:3116:LEU:HD22	1:C:3123:TYR:CD2	2.52	0.44
1:D:4245:ILE:HG13	1:D:4248:TYR:HB2	1.99	0.44
1:A:1231:LEU:O	1:A:1234:GLU:HB3	2.16	0.44
1:B:2167:GLY:C	1:B:2169:ASP:H	2.20	0.44
1:C:3067:HIS:HB3	7:C:5015:HOH:O	2.17	0.44
1:C:3232:VAL:HG11	1:C:3328:VAL:HG22	2.00	0.44
1:D:4017:PRO:HG3	1:D:4183:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4021:PHE:CZ	1:D:4024:ASP:HB2	2.52	0.44
1:D:4225:ARG:HA	1:D:4331:VAL:O	2.17	0.44
1:B:2023:THR:HG22	1:B:2023:THR:O	2.17	0.44
4:G:1:NAG:H62	4:G:2:NAG:C7	2.47	0.44
1:B:2335:ASP:HB3	1:B:2338:THR:OG1	2.18	0.44
1:C:3092:PHE:HB2	1:C:3109:ILE:HD11	1.98	0.44
1:C:3245:ILE:HD11	1:C:3248:TYR:CA	2.47	0.44
1:D:4231:LEU:HD13	1:D:4264:LEU:HD22	2.00	0.44
1:C:3143:GLU:HG3	1:C:3144:GLU:N	2.33	0.44
1:C:3308:TYR:CD1	1:C:3308:TYR:N	2.86	0.44
1:A:1120:GLN:O	1:A:1120:GLN:CG	2.65	0.44
1:B:2200:MET:HE2	1:B:2203:LEU:HD12	1.99	0.44
1:B:2308:TYR:N	1:B:2308:TYR:CD1	2.86	0.44
1:C:3028:GLU:HA	1:C:3035:PHE:CZ	2.52	0.44
1:C:3283:LEU:O	1:C:3297:MET:HA	2.18	0.44
1:D:4162:LEU:HD13	1:D:4194:TRP:CG	2.52	0.44
1:D:4276:PRO:HA	1:D:4277:PRO:HD2	1.93	0.44
1:B:2341:MET:O	1:B:2342:THR:HB	2.17	0.44
1:D:4323:ARG:HA	1:D:4326:GLU:HG2	1.99	0.44
1:A:1232:VAL:HG11	1:A:1328:VAL:HG22	2.00	0.43
1:B:2033:GLN:CB	1:B:2037:GLN:HG2	2.45	0.43
1:C:3107:GLN:O	1:C:3107:GLN:HG3	2.18	0.43
1:D:4224:SER:HB3	1:D:4331:VAL:HG22	2.00	0.43
1:D:4335:ASP:HB3	1:D:4338:THR:OG1	2.18	0.43
1:A:1018:ILE:HD12	1:A:1019:ASP:HB2	2.00	0.43
1:A:1046:HIS:O	1:A:1087:ASN:HA	2.18	0.43
1:C:3006:VAL:HG12	1:C:3060:PHE:CE2	2.47	0.43
1:D:4066:LYS:HD3	1:D:4069:GLN:NE2	2.33	0.43
1:A:1299:TYR:CE2	1:A:1301:ASN:HB3	2.53	0.43
1:A:1040:GLN:NE2	1:B:2100:TRP:HB3	2.34	0.43
1:B:2244:GLN:NE2	1:D:4190:THR:OG1	2.51	0.43
1:C:3093:PRO:O	1:C:3095:GLU:HG2	2.19	0.43
1:C:3204:ARG:O	1:C:3208:GLU:HG3	2.18	0.43
1:D:4103:ILE:H	1:D:4103:ILE:HD12	1.83	0.43
1:D:4191:LEU:HB3	1:D:4195:ALA:HB3	2.00	0.43
1:C:3003:LEU:HD12	1:C:3286:LEU:O	2.17	0.43
1:C:3129:CYS:O	1:C:3133:GLN:HG2	2.18	0.43
1:D:4182:TYR:O	1:D:4186:VAL:HG23	2.19	0.43
1:C:3246:PRO:O	1:C:3247:SER:CB	2.67	0.43
1:B:2258:ASP:O	1:B:2276:PRO:HG2	2.19	0.43
1:A:1221:LYS:HD3	1:A:1331:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2005:PHE:CZ	1:B:2238:HIS:HB3	2.54	0.43
1:B:2006:VAL:HG13	1:B:2251:LEU:HD13	2.01	0.42
1:C:3065:TYR:N	1:C:3092:PHE:CD1	2.87	0.42
1:D:4031:TRP:HA	1:D:4032:PRO:HD2	1.77	0.42
1:A:1206:LEU:HD23	1:A:1206:LEU:HA	1.88	0.42
1:A:1277:PRO:HG2	1:A:1280:SER:HB3	2.01	0.42
1:D:4079:ARG:NH1	6:D:4345:PT3:C3	2.82	0.42
1:A:1082:MET:HE3	1:B:2108:PRO:HG2	2.01	0.42
1:A:1315:CYS:HA	1:A:1323:ARG:HH11	1.84	0.42
1:C:3162:LEU:HD13	1:C:3194:TRP:CB	2.49	0.42
1:A:1188:ASN:HD21	5:A:1371:NAG:H5	1.24	0.42
7:A:5418:HOH:O	1:B:2033:GLN:CG	2.56	0.42
1:B:2017:PRO:HD3	1:B:2031:TRP:CZ2	2.55	0.42
1:C:3221:LYS:NZ	1:C:3330:PRO:HG2	2.35	0.42
1:C:3257:HIS:CD2	1:C:3257:HIS:N	2.88	0.42
1:D:4100:TRP:HE1	1:D:4107:GLN:HA	1.84	0.42
1:D:4200:MET:HE1	1:D:4203:LEU:HD12	2.00	0.42
1:B:2011:ARG:NE	1:B:2258:ASP:HB3	2.33	0.42
1:B:2283:LEU:H	1:B:2283:LEU:CD2	2.32	0.42
1:C:3100:TRP:NE1	1:C:3106:TRP:O	2.52	0.42
1:A:1114:VAL:HG13	1:A:1115:PRO:HD2	2.02	0.42
1:A:1124:LEU:HB3	1:A:1215:TYR:OH	2.20	0.42
1:A:1243:THR:HG22	1:A:1244:GLN:HG3	2.01	0.42
1:B:2149:LEU:HD12	1:B:2149:LEU:O	2.19	0.42
1:C:3191:LEU:HB3	1:C:3195:ALA:HB3	2.01	0.42
1:A:1174:TRP:CH2	1:A:1211:LEU:HD13	2.54	0.42
1:D:4070:VAL:HG21	1:D:4092:PHE:CZ	2.55	0.42
1:B:2132:PHE:HZ	1:B:2214:LEU:CD2	2.33	0.42
1:D:4014:ASP:HA	1:D:4278:TYR:CD1	2.54	0.42
1:D:4257:HIS:CD2	1:D:4257:HIS:N	2.87	0.42
1:D:4258:ASP:HB2	1:D:4276:PRO:HD2	2.01	0.42
1:A:1019:ASP:OD2	1:A:1176:LYS:HE2	2.20	0.42
1:A:1030:SER:CB	1:C:3245:ILE:HB	2.42	0.42
1:D:4062:ASN:O	1:D:4063:GLU:HG3	2.19	0.42
1:D:4167:GLY:C	1:D:4169:ASP:H	2.22	0.42
1:D:4213:SER:HB3	1:D:4217:ILE:HD11	2.01	0.42
1:B:2257:HIS:HB3	6:B:2345:PT3:O2	2.20	0.42
1:D:4005:PHE:HZ	1:D:4252:ILE:HD12	1.84	0.42
1:D:4053:ILE:HG23	1:D:4057:TYR:CE2	2.55	0.42
1:D:4143:GLU:HG3	1:D:4144:GLU:N	2.34	0.42
1:D:4294:PHE:HA	1:D:4319:CYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:LEU:O	1:A:1053:ILE:HG12	2.20	0.41
1:A:1315:CYS:HA	1:A:1323:ARG:NH1	2.35	0.41
1:B:2007:THR:HB	1:B:2284:THR:HG23	2.02	0.41
1:C:3010:PHE:CZ	1:C:3253:MET:HE3	2.55	0.41
1:D:4079:ARG:NH1	6:D:4345:PT3:C4	2.83	0.41
1:C:3005:PHE:HD1	1:C:3249:LYS:O	2.03	0.41
1:C:3100:TRP:HE1	1:C:3107:GLN:HA	1.86	0.41
1:C:3006:VAL:HG21	1:C:3057:TYR:CZ	2.55	0.41
1:C:3012:HIS:CE1	1:C:3015:ARG:HG2	2.54	0.41
1:A:1029:SER:HB2	1:C:3247:SER:HB3	2.01	0.41
1:B:2021:PHE:CE1	1:B:2024:ASP:HB2	2.56	0.41
1:B:2031:TRP:HA	1:B:2032:PRO:HD2	1.78	0.41
1:B:2251:LEU:HD12	1:B:2252:ILE:N	2.35	0.41
1:C:3011:ARG:HG2	1:C:3012:HIS:N	2.34	0.41
1:C:3012:HIS:HE1	1:C:3015:ARG:HG2	1.85	0.41
1:C:3132:PHE:HZ	1:C:3214:LEU:HD23	1.85	0.41
1:C:3135:LEU:HD11	1:C:3222:GLU:HG2	2.02	0.41
1:D:4181:LEU:HD13	1:D:4200:MET:CE	2.51	0.41
1:B:2012:HIS:CD2	6:B:2345:PT3:HO3	2.39	0.41
1:A:1009:VAL:O	1:A:1009:VAL:CG2	2.68	0.41
1:B:2177:VAL:O	1:B:2180:PRO:HD2	2.20	0.41
1:B:2225:ARG:HA	1:B:2331:VAL:O	2.21	0.41
1:C:3006:VAL:HG21	1:C:3057:TYR:OH	2.21	0.41
1:C:3022:PRO:HG2	1:C:3164:GLY:HA3	2.03	0.41
1:C:3236:LEU:CD2	1:C:3240:LYS:HE3	2.51	0.41
1:A:1110:PRO:HG3	1:B:2078:ASP:CG	2.40	0.41
1:A:1132:PHE:HD2	1:A:1133:GLN:NE2	2.18	0.41
1:C:3023:THR:O	1:C:3023:THR:CG2	2.67	0.41
1:C:3031:TRP:HA	1:C:3032:PRO:HD2	1.74	0.41
1:C:3289:GLU:HB3	1:C:3294:PHE:HE1	1.86	0.41
1:D:4312:LEU:HD22	1:D:4324:PHE:CD1	2.56	0.41
1:D:4009:VAL:O	1:D:4009:VAL:CG2	2.69	0.41
1:D:4077:VAL:HG11	1:D:4079:ARG:CZ	2.51	0.41
5:A:1371:NAG:H61	2:E:1:NAG:C1	2.52	0.40
1:B:2322:GLU:H	1:B:2322:GLU:CD	2.25	0.40
1:C:3200:MET:HE2	1:C:3203:LEU:HD12	2.02	0.40
1:D:4162:LEU:HD13	1:D:4194:TRP:HB2	2.03	0.40
1:D:4256:ALA:HB1	1:D:4260:THR:OG1	2.22	0.40
1:C:3180:PRO:O	1:C:3184:GLU:HG3	2.21	0.40
1:D:4049:LEU:O	1:D:4053:ILE:HG12	2.21	0.40
1:D:4184:GLU:HB3	1:D:4189:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:LEU:H	1:A:1283:LEU:CD2	2.34	0.40
1:B:2047:TYR:O	1:B:2051:GLU:HG3	2.22	0.40
1:C:3007:THR:HG21	1:C:3235:ILE:HG12	2.03	0.40
1:D:4131:ARG:O	1:D:4134:GLU:HB3	2.21	0.40
1:A:1246:PRO:O	1:A:1247:SER:HB2	2.22	0.40
1:C:3077:VAL:HG23	1:C:3116:LEU:HD21	2.02	0.40
1:C:3170:LEU:HB3	1:C:3210:SER:HB2	2.04	0.40
1:C:3236:LEU:HD22	1:C:3240:LYS:HE3	2.04	0.40
1:D:4006:VAL:HG21	1:D:4057:TYR:OH	2.21	0.40
1:D:4018:ILE:HD12	1:D:4019:ASP:HB2	2.04	0.40
1:D:4218:HIS:NE2	1:D:4219:LYS:HD2	2.37	0.40
1:D:4329:GLY:N	1:D:4330:PRO:HD2	2.37	0.40
1:A:1070:VAL:HG21	1:A:1092:PHE:CZ	2.56	0.40
1:A:1224:SER:HB3	1:A:1331:VAL:HG22	2.04	0.40
1:B:2010:PHE:CZ	1:B:2253:MET:HE3	2.57	0.40
1:B:2017:PRO:HG3	1:B:2183:CYS:HB2	2.04	0.40
1:B:2299:TYR:HE2	7:B:5299:HOH:O	2.05	0.40
1:C:3131:ARG:CD	1:C:3342:THR:HG21	2.51	0.40
1:D:4017:PRO:HD3	1:D:4031:TRP:CZ2	2.57	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	340/342 (99%)	309 (91%)	27 (8%)	4 (1%)	13 40
1	B	340/342 (99%)	313 (92%)	22 (6%)	5 (2%)	10 34
1	C	340/342 (99%)	306 (90%)	29 (8%)	5 (2%)	10 34
1	D	340/342 (99%)	312 (92%)	22 (6%)	6 (2%)	8 29
All	All	1360/1368 (99%)	1240 (91%)	100 (7%)	20 (2%)	10 34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3218	HIS
1	A	1064	SER
1	A	1218	HIS
1	B	2064	SER
1	C	3064	SER
1	D	4064	SER
1	A	1065	TYR
1	B	2218	HIS
1	C	3121	LEU
1	D	4168	GLN
1	D	4218	HIS
1	C	3065	TYR
1	D	4121	LEU
1	B	2065	TYR
1	B	2121	LEU
1	C	3168	GLN
1	D	4065	TYR
1	B	2217	ILE
1	D	4217	ILE
1	A	1217	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	314/314 (100%)	287 (91%)	27 (9%)	10 30
1	B	314/314 (100%)	287 (91%)	27 (9%)	10 30
1	C	314/314 (100%)	288 (92%)	26 (8%)	11 32
1	D	314/314 (100%)	287 (91%)	27 (9%)	10 30
All	All	1256/1256 (100%)	1149 (92%)	107 (8%)	10 31

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1001	LYS
1	A	1009	VAL
1	A	1015	ARG
1	A	1049	LEU
1	A	1081	LEU
1	A	1091	LEU
1	A	1103	ILE
1	A	1117	SER
1	A	1120	GLN
1	A	1123	TYR
1	A	1147	LYS
1	A	1154	ASP
1	A	1159	LEU
1	A	1165	LEU
1	A	1177	VAL
1	A	1214	LEU
1	A	1231	LEU
1	A	1236	LEU
1	A	1243	THR
1	A	1245	ILE
1	A	1269	ASP
1	A	1283	LEU
1	A	1284	THR
1	A	1304	GLN
1	A	1316	SER
1	A	1328	VAL
1	A	1331	VAL
1	B	2001	LYS
1	B	2009	VAL
1	B	2015	ARG
1	B	2049	LEU
1	B	2081	LEU
1	B	2091	LEU
1	B	2103	ILE
1	B	2115	PRO
1	B	2117	SER
1	B	2147	LYS
1	B	2154	ASP
1	B	2159	LEU
1	B	2177	VAL
1	B	2197	GLU
1	B	2214	LEU
1	B	2231	LEU

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Mol	Chain	Res	Type
1	B	2236	LEU
1	B	2243	THR
1	B	2245	ILE
1	B	2269	ASP
1	B	2283	LEU
1	B	2284	THR
1	B	2304	GLN
1	B	2316	SER
1	B	2323	ARG
1	B	2328	VAL
1	B	2331	VAL
1	C	3001	LYS
1	C	3009	VAL
1	C	3015	ARG
1	C	3049	LEU
1	C	3081	LEU
1	C	3091	LEU
1	C	3103	ILE
1	C	3117	SER
1	C	3147	LYS
1	C	3154	ASP
1	C	3159	LEU
1	C	3177	VAL
1	C	3197	GLU
1	C	3214	LEU
1	C	3231	LEU
1	C	3236	LEU
1	C	3243	THR
1	C	3245	ILE
1	C	3269	ASP
1	C	3283	LEU
1	C	3284	THR
1	C	3304	GLN
1	C	3305	HIS
1	C	3316	SER
1	C	3328	VAL
1	C	3331	VAL
1	D	4001	LYS
1	D	4009	VAL
1	D	4015	ARG
1	D	4049	LEU
1	D	4081	LEU

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Mol	Chain	Res	Type
1	D	4091	LEU
1	D	4103	ILE
1	D	4117	SER
1	D	4123	TYR
1	D	4147	LYS
1	D	4154	ASP
1	D	4159	LEU
1	D	4177	VAL
1	D	4197	GLU
1	D	4214	LEU
1	D	4231	LEU
1	D	4236	LEU
1	D	4243	THR
1	D	4245	ILE
1	D	4269	ASP
1	D	4283	LEU
1	D	4284	THR
1	D	4304	GLN
1	D	4308	TYR
1	D	4316	SER
1	D	4328	VAL
1	D	4331	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1033	GLN
1	A	1037	GLN
1	A	1040	GLN
1	A	1069	GLN
1	A	1187	HIS
1	A	1233	ASN
1	A	1237	ASN
1	A	1265	GLN
1	B	2040	GLN
1	B	2120	GLN
1	B	2233	ASN
1	B	2237	ASN
1	B	2244	GLN
1	B	2265	GLN
1	B	2305	HIS
1	C	3120	GLN

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Mol	Chain	Res	Type
1	C	3237	ASN
1	C	3244	GLN
1	C	3265	GLN
1	D	4168	GLN
1	D	4187	HIS
1	D	4233	ASN
1	D	4237	ASN
1	D	4244	GLN
1	D	4265	GLN
1	D	4305	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 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	14,14,15	1.67	2 (14%)	17,19,21	1.36	2 (11%)
2	BMA	E	2	2	11,11,12	2.57	4 (36%)	15,15,17	1.05	2 (13%)
2	MAN	E	3	2	11,11,12	2.38	4 (36%)	15,15,17	1.10	1 (6%)
3	NAG	F	1	1,3	14,14,15	1.45	2 (14%)	17,19,21	1.56	2 (11%)
3	NAG	F	2	3	14,14,15	1.59	1 (7%)	17,19,21	1.63	2 (11%)
4	NAG	G	1	1,4	14,14,15	1.77	3 (21%)	17,19,21	1.79	4 (23%)
4	NAG	G	2	4	14,14,15	1.89	3 (21%)	17,19,21	1.72	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BMA	G	3	4	11,11,12	2.31	4 (36%)	15,15,17	1.20	2 (13%)

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

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	BMA	C4-C5	5.95	1.65	1.53
4	G	2	NAG	C4-C5	5.50	1.64	1.53
2	E	1	NAG	C4-C5	4.94	1.63	1.53
4	G	3	BMA	C4-C5	4.88	1.63	1.53
3	F	2	NAG	C4-C5	4.86	1.63	1.53
4	G	1	NAG	C4-C5	4.82	1.63	1.53
2	E	3	MAN	O5-C5	4.39	1.52	1.43
2	E	3	MAN	C4-C5	4.25	1.62	1.53
2	E	2	BMA	O5-C5	3.99	1.51	1.43
4	G	3	BMA	O5-C5	3.79	1.50	1.43
3	F	1	NAG	C4-C5	3.77	1.61	1.53
4	G	1	NAG	O5-C1	-2.77	1.39	1.43
3	F	1	NAG	O5-C1	-2.69	1.39	1.43
2	E	1	NAG	C6-C5	2.57	1.60	1.51
2	E	3	MAN	O5-C1	2.39	1.47	1.43
2	E	2	BMA	C6-C5	2.38	1.59	1.51
2	E	3	MAN	C6-C5	2.36	1.59	1.51
4	G	3	BMA	C6-C5	2.23	1.59	1.51
4	G	2	NAG	O5-C1	-2.17	1.40	1.43
4	G	3	BMA	O5-C1	2.12	1.47	1.43
2	E	2	BMA	C2-C3	2.04	1.55	1.52
4	G	1	NAG	C1-C2	2.03	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	NAG	C3-C2	-2.03	1.48	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2	NAG	C2-N2-C7	-5.11	116.05	122.90
4	G	1	NAG	C1-O5-C5	4.89	118.74	112.19
3	F	2	NAG	C2-N2-C7	-4.32	117.10	122.90
3	F	1	NAG	C1-O5-C5	4.05	117.61	112.19
3	F	2	NAG	C1-O5-C5	3.93	117.46	112.19
2	E	1	NAG	C2-N2-C7	-3.44	118.29	122.90
4	G	1	NAG	C2-N2-C7	-3.37	118.39	122.90
2	E	1	NAG	C1-O5-C5	3.15	116.41	112.19
4	G	3	BMA	O2-C2-C3	-2.63	104.70	110.15
4	G	2	NAG	C4-C3-C2	-2.41	107.49	111.02
4	G	1	NAG	O5-C5-C6	-2.36	103.07	107.66
4	G	2	NAG	C1-O5-C5	2.28	115.24	112.19
3	F	1	NAG	O5-C1-C2	-2.27	107.78	111.29
4	G	3	BMA	C1-C2-C3	2.26	112.93	109.64
2	E	2	BMA	O2-C2-C3	-2.18	105.64	110.15
2	E	3	MAN	O2-C2-C3	-2.16	105.68	110.15
2	E	2	BMA	O6-C6-C5	2.11	118.53	111.33
4	G	1	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	BMA	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6

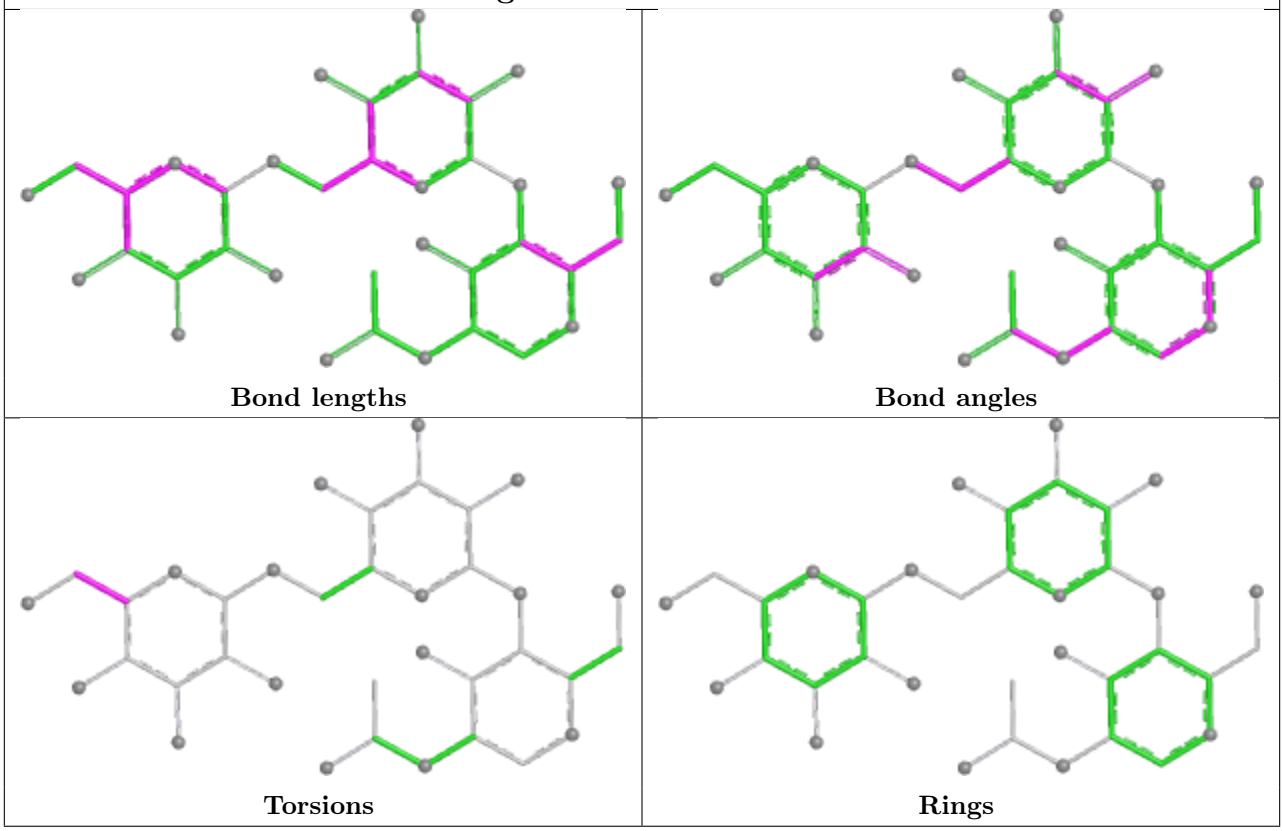
There are no ring outliers.

4 monomers are involved in 9 short contacts:

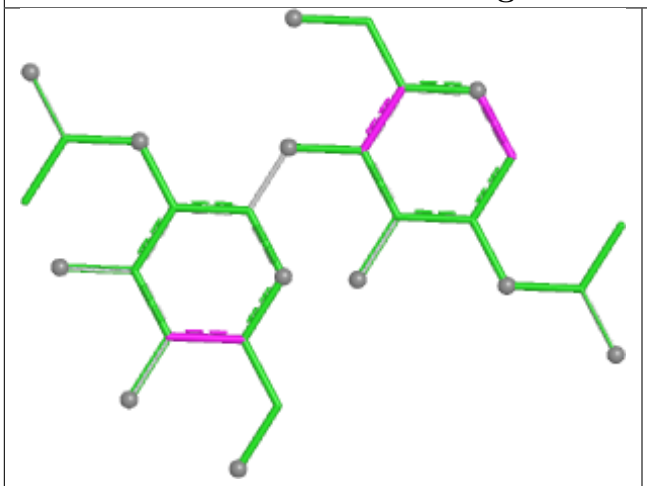
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	BMA	2	0
2	E	1	NAG	2	0
4	G	1	NAG	6	0
4	G	2	NAG	3	0

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

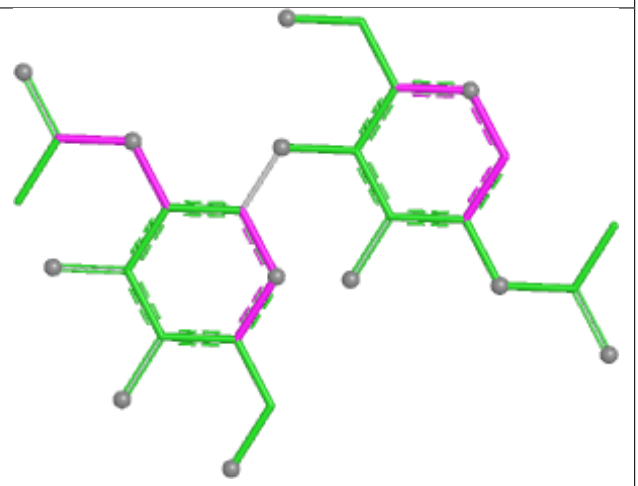
Oligosaccharide Chain E



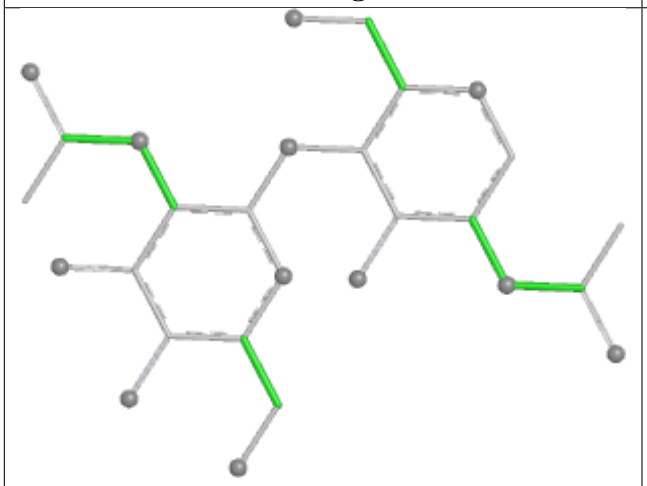
Oligosaccharide Chain F



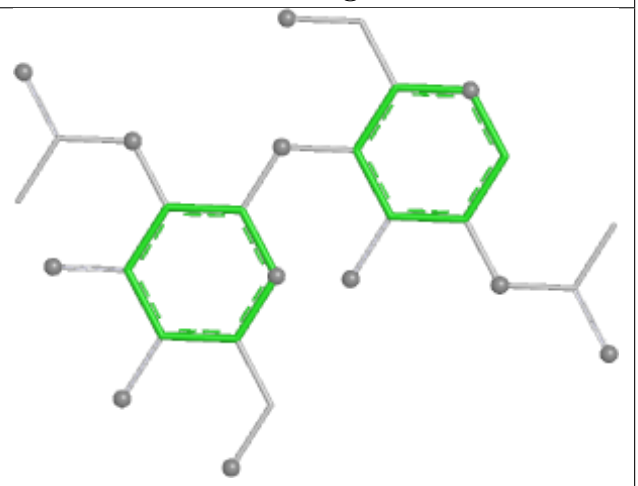
Bond lengths



Bond angles

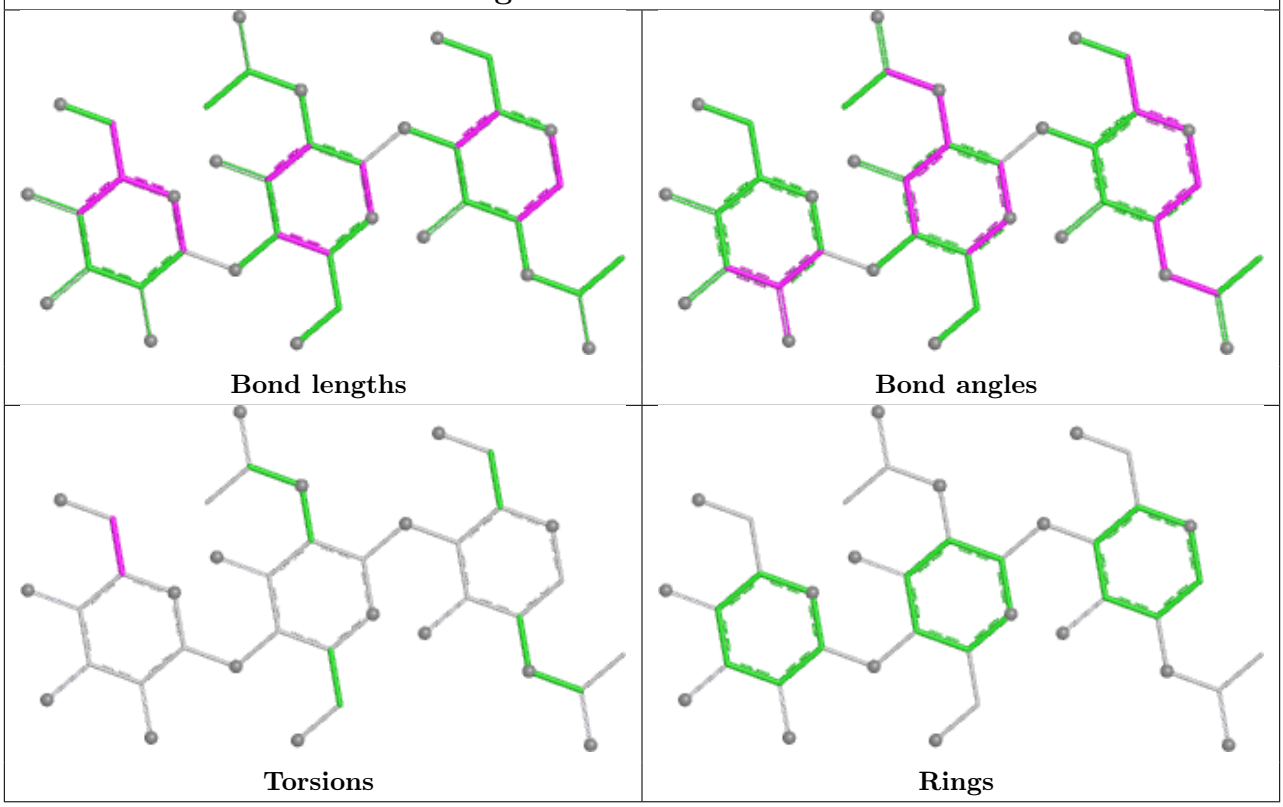


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

8 ligands 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	$\#\|Z\| > 2$
5	NAG	C	3371	1	14,14,15	1.84	3 (21%)	17,19,21	1.06	1 (5%)
5	NAG	A	1371	1	14,14,15	1.76	3 (21%)	17,19,21	1.51	2 (11%)
5	NAG	B	2381	1	14,14,15	1.73	2 (14%)	17,19,21	1.82	4 (23%)
5	NAG	C	3381	1	14,14,15	1.93	3 (21%)	17,19,21	1.67	3 (17%)
6	PT3	B	2345	-	12,12,12	1.72	3 (25%)	15,15,15	1.60	4 (26%)
5	NAG	C	3361	1	14,14,15	4.63	8 (57%)	17,19,21	2.62	8 (47%)
6	PT3	D	4345	-	12,12,12	1.78	2 (16%)	15,15,15	1.75	4 (26%)
6	PT3	A	1345	-	12,12,12	1.30	1 (8%)	15,15,15	1.86	5 (33%)

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	C	3371	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1371	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	2381	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3381	1	-	0/6/23/26	0/1/1/1
6	PT3	B	2345	-	-	4/16/16/16	-
5	NAG	C	3361	1	-	0/6/23/26	0/1/1/1
6	PT3	D	4345	-	-	4/16/16/16	-
6	PT3	A	1345	-	-	4/16/16/16	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3361	NAG	O5-C1	-11.37	1.24	1.43
5	C	3361	NAG	C1-C2	9.64	1.65	1.52
5	C	3381	NAG	C4-C5	5.32	1.64	1.53
5	B	2381	NAG	C4-C5	5.28	1.64	1.53
5	A	1371	NAG	C4-C5	5.10	1.63	1.53
5	C	3371	NAG	C4-C5	4.82	1.63	1.53
6	D	4345	PT3	C2-C1	4.18	1.58	1.52
5	C	3361	NAG	C4-C3	3.97	1.62	1.52
6	B	2345	PT3	C2-C1	3.78	1.58	1.52
5	C	3361	NAG	C8-C7	3.59	1.58	1.50
6	D	4345	PT3	O41-C4	-3.55	1.16	1.23
5	C	3361	NAG	O6-C6	3.31	1.56	1.42
5	C	3361	NAG	C6-C5	3.31	1.62	1.51
5	C	3361	NAG	C4-C5	3.02	1.59	1.53
5	C	3361	NAG	O5-C5	-2.93	1.37	1.43
6	B	2345	PT3	O3-C3	2.82	1.47	1.42
6	A	1345	PT3	O41-C4	-2.80	1.18	1.23
5	C	3371	NAG	O5-C1	-2.66	1.39	1.43
5	A	1371	NAG	C6-C5	2.48	1.60	1.51
5	A	1371	NAG	O5-C1	-2.44	1.39	1.43
6	B	2345	PT3	O41-C4	-2.43	1.18	1.23
5	B	2381	NAG	C6-C5	2.38	1.59	1.51
5	C	3381	NAG	C1-C2	2.22	1.55	1.52
5	C	3381	NAG	C4-C3	2.11	1.57	1.52
5	C	3371	NAG	C1-C2	2.10	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	3361	NAG	C1-O5-C5	5.23	119.19	112.19
5	B	2381	NAG	C1-O5-C5	4.67	118.44	112.19
5	C	3361	NAG	C4-C3-C2	-4.56	104.33	111.02
5	A	1371	NAG	C2-N2-C7	-4.08	117.44	122.90
6	A	1345	PT3	O2-C2-C1	-3.92	102.31	110.69
5	C	3381	NAG	C1-O5-C5	3.82	117.31	112.19
5	C	3361	NAG	C1-C2-N2	-3.81	104.43	110.43
5	C	3361	NAG	C2-N2-C7	-3.81	117.79	122.90
5	C	3381	NAG	O5-C1-C2	-3.68	105.59	111.29
6	D	4345	PT3	C41-N4-C4	-3.67	115.95	122.55
6	A	1345	PT3	C41-N4-C4	-3.53	116.20	122.55
5	B	2381	NAG	C2-N2-C7	-3.38	118.37	122.90
5	B	2381	NAG	O5-C1-C2	-3.31	106.17	111.29
5	A	1371	NAG	C1-O5-C5	3.10	116.34	112.19
6	D	4345	PT3	O2-C2-C1	-3.01	104.26	110.69
6	D	4345	PT3	O41-C4-C3	2.96	125.21	119.99
6	B	2345	PT3	C41-N4-C4	-2.94	117.27	122.55
6	B	2345	PT3	O2-C2-C1	-2.81	104.68	110.69
6	B	2345	PT3	O41-C4-C3	2.80	124.93	119.99
5	C	3361	NAG	C3-C4-C5	2.78	115.27	110.23
5	C	3361	NAG	O5-C5-C4	-2.68	104.30	110.83
6	B	2345	PT3	C3-C4-N4	-2.65	111.37	116.64
5	C	3361	NAG	O3-C3-C4	2.61	116.54	110.38
5	C	3371	NAG	C8-C7-N2	-2.53	111.93	116.12
5	C	3381	NAG	C8-C7-N2	-2.35	112.22	116.12
6	D	4345	PT3	C3-C4-N4	-2.33	112.01	116.64
5	B	2381	NAG	C8-C7-N2	-2.17	112.53	116.12
6	A	1345	PT3	C3-C2-C1	-2.11	105.16	109.82
6	A	1345	PT3	C3-C4-N4	-2.04	112.59	116.64
5	C	3361	NAG	C6-C5-C4	-2.03	108.03	113.02
6	A	1345	PT3	O1-C1-O11	2.01	128.64	124.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1371	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1345	PT3	O3-C3-C4-N4

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Mol	Chain	Res	Type	Atoms
6	D	4345	PT3	O3-C3-C4-O41
6	A	1345	PT3	C2-C3-C4-O41
6	A	1345	PT3	C2-C3-C4-N4
6	B	2345	PT3	C2-C3-C4-N4
6	B	2345	PT3	C2-C3-C4-O41
6	D	4345	PT3	O3-C3-C4-N4
6	A	1345	PT3	O3-C3-C4-O41
6	B	2345	PT3	O3-C3-C4-O41
6	D	4345	PT3	C2-C3-C4-O41
6	B	2345	PT3	O3-C3-C4-N4
6	D	4345	PT3	C2-C3-C4-N4

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3371	NAG	1	0
5	A	1371	NAG	4	0
6	B	2345	PT3	6	0
5	C	3361	NAG	1	0
6	D	4345	PT3	6	0
6	A	1345	PT3	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.