Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 04:12 PM EST

PDB ID	:	8API
Title	:	THE S VARIANT OF HUMAN ALPHA1-ANTITRYPSIN, STRUCTURE AND IMPLICATIONS FOR FUNCTION AND METABOLISM
Authors	:	Loebermann, H.; Tokuoka, R.; Deisenhofer, J.; Huber, R.
Deposited on	:	1988-09-08
Resolution	:	3.10 Å(reported)

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

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

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

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

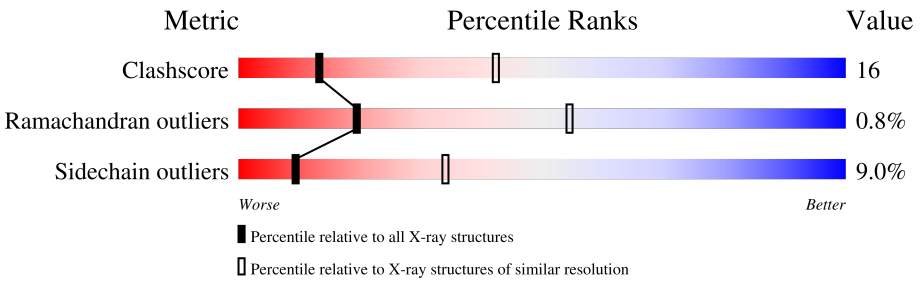
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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	347	54% 35% 7% • •
2	B	36	47% 44% 8%
3	C	6	100%
4	D	2	100%
4	E	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	1	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3286 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.

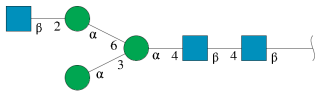
- Molecule 1 is a protein called ALPHA-1 ANTITRYPSIN (CHAIN A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2698	1730	442	518	8	7	0	0

- Molecule 2 is a protein called ALPHA-1 ANTITRYPSIN (CHAIN B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	36	291	193	46	50	2	5	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-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
			Total	C	N	O			
3	C	6	75	42	3	30	44	0	0

- Molecule 4 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			
4	D	2	28	16	2	10	14	0	0

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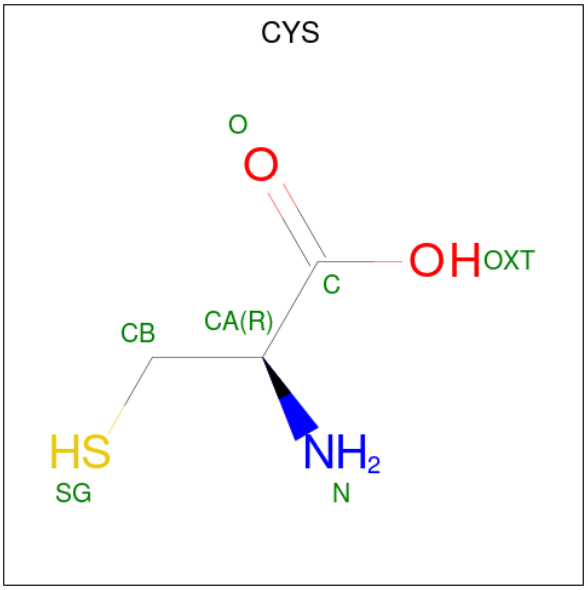
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	28	16	2	10	0	0	0

- Molecule 5 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	7	3	1	2	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	137	137	137	0	0
			Total	O		
6	B	22	22	22	0	0

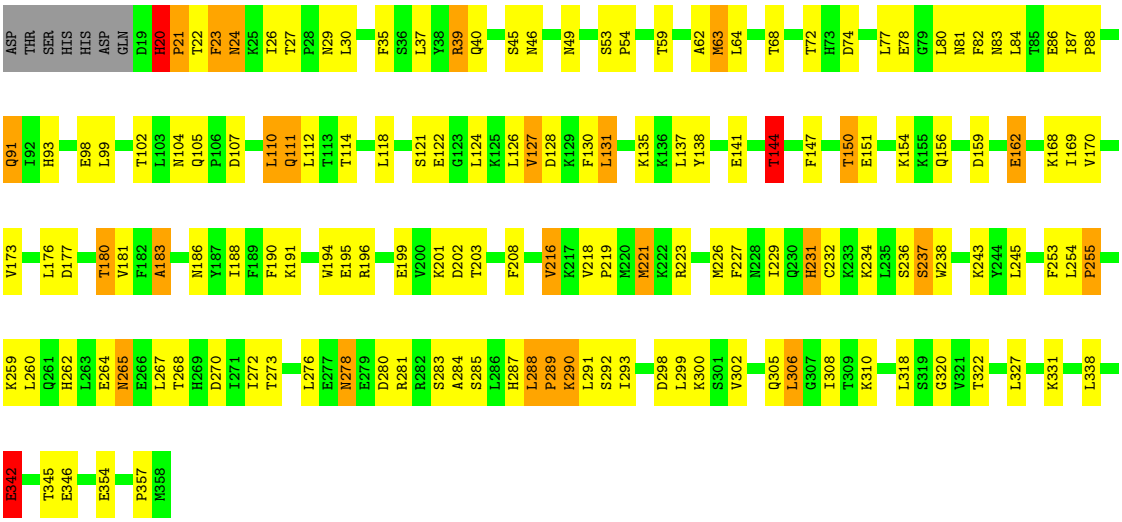
3 Residue-property plots (i)

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: ALPHA-1 ANTITRYPSIN (CHAIN A)

Chain A: 54% 35% 7%



• Molecule 2: ALPHA-1 ANTITRYPSIN (CHAIN B)

Chain B: 47% 44% 8%

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

Chain C: 100%

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

Chain D: 100%

NAG1
NAG2

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

Chain E: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.70Å 119.70Å 216.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3286	wwPDB-VP
Average B, all atoms ($Å^2$)	16.0	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: NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.94	3/2752 (0.1%)	1.45	9/3718 (0.2%)
2	B	0.93	0/299	1.35	0/402
All	All	0.94	3/3051 (0.1%)	1.44	9/4120 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	28

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	TRP	NE1-CE2	-7.63	1.27	1.37
1	A	238	TRP	NE1-CE2	-7.36	1.27	1.37
1	A	231	HIS	CE1-NE2	5.09	1.44	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	183	ALA	CB-CA-C	-6.55	100.28	110.10
1	A	278	ASN	CA-CB-CG	-6.50	99.11	113.40
1	A	39	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	237	SER	CB-CA-C	-6.28	98.17	110.10
1	A	292	SER	N-CA-CB	5.90	119.35	110.50
1	A	338	LEU	N-CA-CB	-5.57	99.27	110.40
1	A	292	SER	CB-CA-C	-5.55	99.55	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	LEU	N-CA-CB	-5.39	99.62	110.40

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LEU	Mainchain
1	A	127	VAL	Mainchain
1	A	144	THR	Mainchain
1	A	159	ASP	Mainchain
1	A	162	GLU	Mainchain
1	A	169	ILE	Mainchain
1	A	180	THR	Mainchain
1	A	183	ALA	Mainchain
1	A	196	ARG	Mainchain
1	A	203	THR	Mainchain
1	A	21	PRO	Mainchain,Peptide
1	A	226	MET	Mainchain
1	A	231	HIS	Mainchain
1	A	237	SER	Mainchain
1	A	24	ASN	Mainchain
1	A	255	PRO	Mainchain
1	A	289	PRO	Mainchain
1	A	290	LYS	Mainchain
1	A	291	LEU	Mainchain
1	A	298	ASP	Mainchain,Peptide
1	A	300	LYS	Mainchain
1	A	308	ILE	Mainchain
1	A	342	GLU	Mainchain
1	A	345	THR	Mainchain
1	A	46	ASN	Sidechain
1	A	63	MET	Mainchain

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	2698	0	2689	87	0
2	B	291	0	306	22	0
3	C	75	0	64	0	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	7	0	3	1	0
6	A	137	0	0	0	1
6	B	22	0	0	0	0
All	All	3286	0	3112	99	1

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 (99) 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:162:GLU:HG3	1:A:170:VAL:HG12	1.67	0.77
1:A:110:LEU:HD11	1:A:190:PHE:HE1	1.52	0.75
1:A:93:HIS:HB3	1:A:137:LEU:HD23	1.69	0.74
1:A:77:LEU:HD23	1:A:84:LEU:HD21	1.69	0.73
1:A:88:PRO:HB2	1:A:91:GLN:HB2	1.70	0.72
1:A:208:PHE:HB2	1:A:218:VAL:HG21	1.73	0.68
1:A:195:GLU:HA	1:A:245:LEU:HD21	1.77	0.65
1:A:195:GLU:HA	1:A:245:LEU:CD2	2.26	0.65
1:A:104:ASN:HD21	1:A:114:THR:H	1.45	0.64
1:A:83:ASN:HD22	1:A:86:GLU:HG3	1.61	0.64
1:A:223:ARG:HB3	1:A:227:PHE:HZ	1.65	0.62
1:A:236:SER:HB2	1:A:262:HIS:HD2	1.63	0.62
1:A:232:CYS:HB3	1:A:234:LYS:HB2	1.82	0.61
1:A:278:ASN:ND2	1:A:280:ASP:HB2	2.16	0.61
1:A:114:THR:HG22	1:A:188:ILE:HB	1.84	0.60
1:A:195:GLU:HG3	1:A:243:LYS:HB2	1.84	0.60
1:A:283:SER:O	2:B:361:PRO:HB3	2.01	0.60
1:A:331:LYS:HB2	1:A:354:GLU:HG2	1.84	0.58
1:A:83:ASN:O	1:A:87:ILE:HG22	2.04	0.58
1:A:49:ASN:H	2:B:393:GLN:HE22	1.51	0.57
1:A:102:THR:HA	1:A:105:GLN:HG3	1.86	0.57
1:A:219:PRO:HG2	1:A:290:LYS:HB3	1.87	0.57
1:A:287:HIS:HB2	2:B:365:LYS:HA	1.86	0.57
1:A:322:THR:HG22	1:A:327:LEU:HD11	1.86	0.56
1:A:255:PRO:HG3	1:A:260:LEU:HD13	1.86	0.56
1:A:53:SER:HB2	2:B:384:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:GLU:HB2	2:B:383:LEU:HD13	1.89	0.54
1:A:265:ASN:N	1:A:265:ASN:HD22	2.06	0.54
1:A:74:ASP:O	1:A:78:GLU:HB2	2.08	0.54
1:A:37:LEU:HA	1:A:306:LEU:HD11	1.90	0.53
1:A:285:SER:HB3	2:B:363:GLU:HA	1.90	0.53
1:A:130:PHE:HB2	1:A:320:GLY:O	2.08	0.53
2:B:367:ASN:HD22	2:B:368:LYS:HG2	1.73	0.53
1:A:62:ALA:HB1	1:A:138:TYR:OH	2.09	0.53
1:A:23:PHE:HD2	1:A:98:GLU:HB3	1.75	0.52
1:A:181:VAL:HG23	1:A:357:PRO:HD3	1.92	0.52
1:A:49:ASN:H	2:B:393:GLN:NE2	2.07	0.52
1:A:20:HIS:CG	1:A:21:PRO:HD3	2.45	0.51
1:A:24:ASN:HA	1:A:27:THR:HB	1.91	0.51
4:E:1:NAG:H62	4:E:2:NAG:N2	2.24	0.51
2:B:367:ASN:ND2	2:B:368:LYS:HG2	2.25	0.51
1:A:80:LEU:HB3	1:A:82:PHE:HE1	1.76	0.51
1:A:278:ASN:HD21	1:A:280:ASP:HB2	1.77	0.50
2:B:374:MET:HB2	2:B:384:PHE:HB2	1.94	0.49
1:A:254:LEU:HB2	2:B:366:PHE:CE2	2.48	0.49
1:A:191:LYS:HG3	1:A:346:GLU:HB3	1.95	0.49
1:A:162:GLU:CG	1:A:170:VAL:HG12	2.40	0.48
1:A:173:VAL:HG11	1:A:176:LEU:HD12	1.95	0.48
1:A:35:PHE:O	1:A:39:ARG:HG3	2.13	0.48
1:A:110:LEU:HD11	1:A:190:PHE:CE1	2.39	0.48
1:A:199:GLU:HB3	1:A:201:LYS:HD2	1.96	0.47
1:A:208:PHE:HB3	1:A:216:VAL:HG12	1.97	0.47
1:A:284:ALA:HA	2:B:361:PRO:HB2	1.96	0.47
1:A:168:LYS:HD2	1:A:346:GLU:OE1	2.14	0.47
2:B:373:LEU:HD12	2:B:375:ILE:HG13	1.98	0.46
1:A:53:SER:HB2	2:B:384:PHE:CE1	2.50	0.46
1:A:111:GLN:HG3	1:A:191:LYS:HB3	1.98	0.46
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.68	0.46
1:A:284:ALA:HA	2:B:361:PRO:CB	2.45	0.45
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.63	0.45
1:A:288:LEU:HD12	1:A:289:PRO:HD2	1.98	0.45
1:A:264:GLU:C	1:A:265:ASN:HD22	2.19	0.45
1:A:80:LEU:HB3	1:A:82:PHE:CE1	2.52	0.45
2:B:374:MET:O	2:B:383:LEU:HB2	2.17	0.45
1:A:272:ILE:O	1:A:276:LEU:HD13	2.16	0.45
1:A:121:SER:HB2	1:A:147:PHE:HD2	1.82	0.44
2:B:369:PRO:HB3	2:B:389:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:O	1:A:154:LYS:HB2	2.17	0.44
1:A:268:THR:HG22	1:A:270:ASP:H	1.82	0.44
1:A:63:MET:HB3	1:A:138:TYR:CG	2.52	0.44
1:A:156:GLN:HE21	1:A:156:GLN:HB2	1.46	0.44
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.71	0.44
1:A:177:ASP:HB3	1:A:180:THR:OG1	2.17	0.44
1:A:254:LEU:HD12	1:A:255:PRO:HD2	2.01	0.43
1:A:111:GLN:H	1:A:111:GLN:HG2	1.46	0.43
1:A:72:THR:HG22	1:A:310:LYS:HB3	2.00	0.43
1:A:342:GLU:H	1:A:342:GLU:HG2	1.39	0.43
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.85	0.42
2:B:376:GLU:HB3	2:B:379:THR:HG1	1.82	0.42
1:A:26:ILE:O	1:A:29:ASN:HB2	2.19	0.42
1:A:107:ASP:HB3	1:A:110:LEU:O	2.19	0.42
1:A:234:LYS:HG3	5:A:395:CYS:SG	2.60	0.42
1:A:281:ARG:HH11	1:A:281:ARG:HD2	1.70	0.42
1:A:53:SER:HA	1:A:54:PRO:HD3	1.76	0.42
1:A:124:LEU:HD23	1:A:126:LEU:HD21	2.02	0.42
1:A:131:LEU:HD21	1:A:135:LYS:HE3	2.02	0.42
1:A:40:GLN:HB3	1:A:302:VAL:HG13	2.00	0.41
2:B:381:SER:HA	2:B:382:PRO:HD2	1.72	0.41
1:A:114:THR:HG22	1:A:188:ILE:CB	2.48	0.41
1:A:122:GLU:HB3	1:A:144:THR:HG22	2.02	0.41
1:A:63:MET:HB3	1:A:138:TYR:CD2	2.56	0.41
1:A:285:SER:OG	2:B:363:GLU:HG3	2.21	0.41
1:A:318:LEU:HD13	1:A:327:LEU:HB2	2.02	0.41
1:A:229:ILE:HG21	1:A:229:ILE:HD13	1.84	0.41
2:B:360:ILE:HG21	2:B:360:ILE:HD13	1.81	0.41
1:A:253:PHE:O	1:A:255:PRO:HD3	2.21	0.40
2:B:367:ASN:HD22	2:B:367:ASN:C	2.25	0.40
1:A:293:ILE:HG21	1:A:293:ILE:HD13	1.86	0.40
1:A:221:MET:HG3	1:A:288:LEU:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:612:HOH:O	6:A:612:HOH:O[12_564]	0.71	1.49

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	338/347 (97%)	317 (94%)	18 (5%)	3 (1%)	17 52
2	B	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
All	All	372/383 (97%)	349 (94%)	20 (5%)	3 (1%)	19 54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	81	ASN
1	A	127	VAL

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	298/305 (98%)	271 (91%)	27 (9%)	9 33
2	B	35/35 (100%)	32 (91%)	3 (9%)	10 37
All	All	333/340 (98%)	303 (91%)	30 (9%)	9 34

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	22	THR
1	A	23	PHE

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Mol	Chain	Res	Type
1	A	45	SER
1	A	59	THR
1	A	68	THR
1	A	91	GLN
1	A	99	LEU
1	A	110	LEU
1	A	111	GLN
1	A	118	LEU
1	A	128	ASP
1	A	131	LEU
1	A	141	GLU
1	A	144	THR
1	A	150	THR
1	A	151	GLU
1	A	186	ASN
1	A	202	ASP
1	A	216	VAL
1	A	221	MET
1	A	265	ASN
1	A	267	LEU
1	A	273	THR
1	A	305	GLN
1	A	306	LEU
1	A	342	GLU
2	B	367	ASN
2	B	368	LYS
2	B	374	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	97	GLN
1	A	104	ASN
1	A	109	GLN
1	A	111	GLN
1	A	156	GLN
1	A	212	GLN
1	A	261	GLN
1	A	262	HIS
1	A	265	ASN
1	A	287	HIS

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Mol	Chain	Res	Type
2	B	367	ASN
2	B	377	GLN
2	B	378	ASN
2	B	393	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	1.03	2 (14%)	17,19,21	2.07	6 (35%)
3	NAG	C	2	3	14,14,15	1.07	1 (7%)	17,19,21	1.85	3 (17%)
3	MAN	C	3	3	11,11,12	0.90	0	15,15,17	1.76	2 (13%)
3	MAN	C	4	3	11,11,12	1.06	0	15,15,17	2.18	3 (20%)
3	NAG	C	5	3	14,14,15	0.72	0	17,19,21	2.08	2 (11%)
3	MAN	C	6	3	11,11,12	0.59	0	15,15,17	1.64	1 (6%)
4	NAG	D	1	1,4	14,14,15	1.04	1 (7%)	17,19,21	1.33	2 (11%)
4	NAG	D	2	4	14,14,15	0.63	0	17,19,21	1.39	2 (11%)
4	NAG	E	1	1,4	14,14,15	1.26	2 (14%)	17,19,21	2.55	8 (47%)
4	NAG	E	2	4	14,14,15	1.13	1 (7%)	17,19,21	1.90	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	1/6/23/26	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	3.63	1.57	1.52
4	E	2	NAG	C1-C2	2.69	1.56	1.52
3	C	2	NAG	C1-C2	2.30	1.55	1.52
3	C	1	NAG	C3-C2	2.18	1.57	1.52
4	E	1	NAG	C2-N2	2.10	1.49	1.46
4	D	1	NAG	C1-C2	2.07	1.55	1.52
3	C	1	NAG	C1-C2	2.03	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5	NAG	C1-O5-C5	7.46	122.30	112.19
3	C	4	MAN	C1-O5-C5	6.53	121.04	112.19
3	C	2	NAG	C1-O5-C5	6.27	120.69	112.19
4	E	1	NAG	C1-C2-N2	5.83	120.44	110.49
3	C	3	MAN	C1-O5-C5	5.77	120.00	112.19
3	C	6	MAN	C1-O5-C5	5.67	119.87	112.19
3	C	1	NAG	C1-O5-C5	5.50	119.65	112.19
4	E	2	NAG	C1-O5-C5	4.94	118.88	112.19
4	D	2	NAG	C1-O5-C5	4.06	117.70	112.19
4	E	1	NAG	C2-N2-C7	3.91	128.47	122.90
4	E	2	NAG	C2-N2-C7	3.54	127.94	122.90
4	E	1	NAG	O5-C5-C6	3.48	112.66	107.20
4	E	1	NAG	O7-C7-N2	3.27	127.97	121.95
4	E	1	NAG	O7-C7-C8	-3.14	116.22	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2	NAG	C1-C2-N2	3.10	115.79	110.49
4	E	1	NAG	O5-C1-C2	-3.08	106.42	111.29
4	D	1	NAG	C1-O5-C5	2.96	116.20	112.19
3	C	1	NAG	C3-C4-C5	2.74	115.13	110.24
3	C	1	NAG	C4-C3-C2	2.70	114.98	111.02
3	C	4	MAN	O2-C2-C1	-2.66	103.71	109.15
4	E	1	NAG	C4-C3-C2	2.46	114.62	111.02
3	C	3	MAN	O5-C1-C2	-2.45	107.00	110.77
4	D	1	NAG	O7-C7-N2	2.39	126.35	121.95
4	D	2	NAG	O5-C1-C2	-2.36	107.56	111.29
3	C	2	NAG	O7-C7-N2	2.33	126.23	121.95
4	E	2	NAG	O7-C7-N2	2.28	126.14	121.95
3	C	1	NAG	O7-C7-N2	2.25	126.10	121.95
4	E	1	NAG	C1-O5-C5	2.25	115.24	112.19
3	C	1	NAG	O5-C1-C2	-2.23	107.77	111.29
3	C	5	NAG	O7-C7-N2	2.15	125.91	121.95
3	C	4	MAN	O5-C1-C2	-2.14	107.46	110.77
3	C	1	NAG	C2-N2-C7	2.06	125.84	122.90
3	C	2	NAG	O7-C7-C8	-2.00	118.34	122.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	1	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
3	C	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7
3	C	5	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7

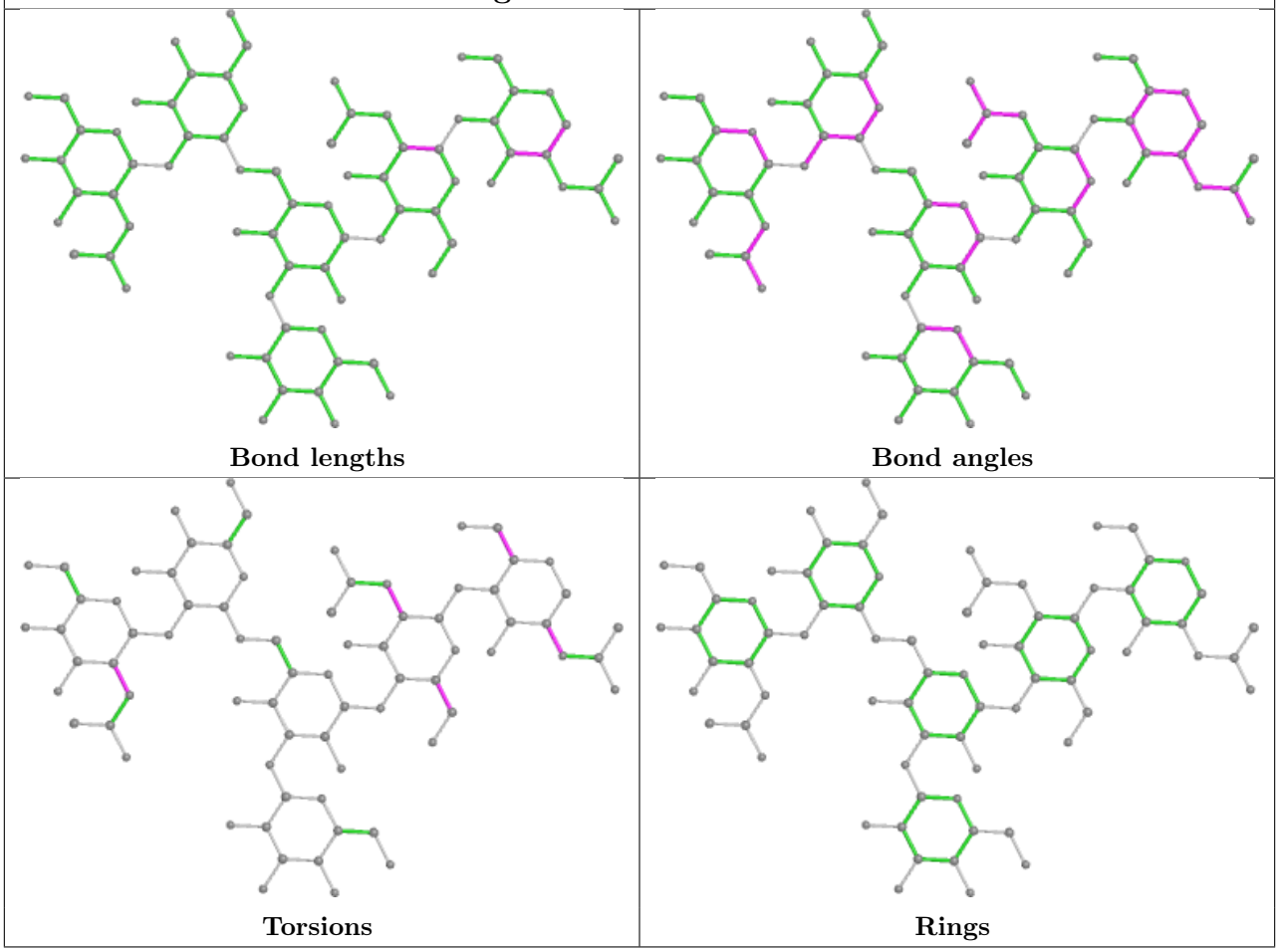
There are no ring outliers.

2 monomers are involved in 1 short contact:

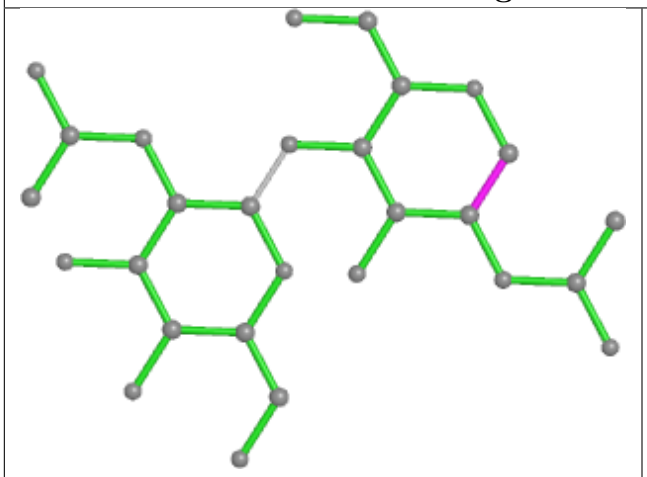
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
4	E	2	NAG	1	0

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

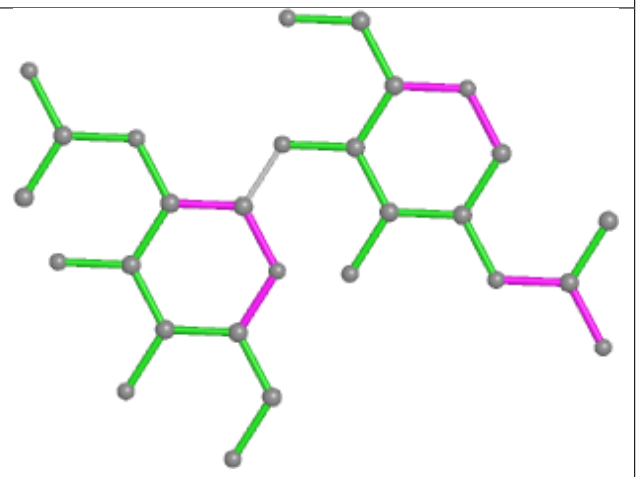
Oligosaccharide Chain C



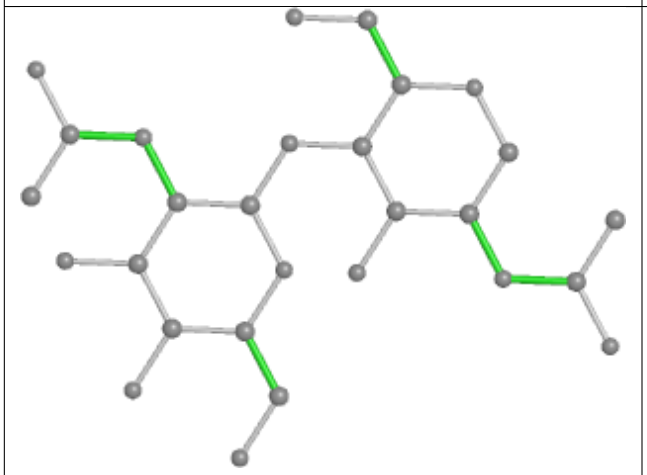
Oligosaccharide Chain D



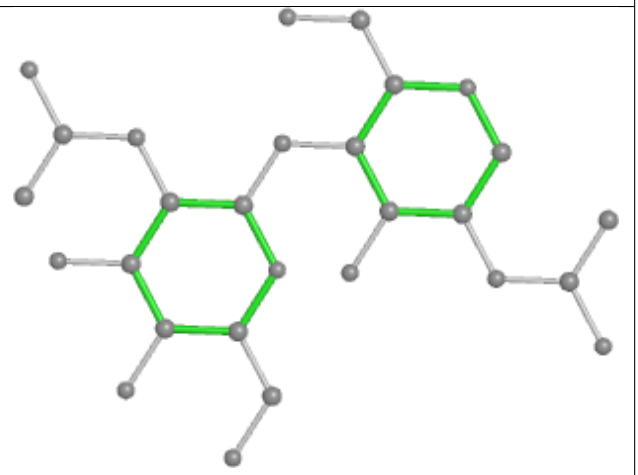
Bond lengths



Bond angles

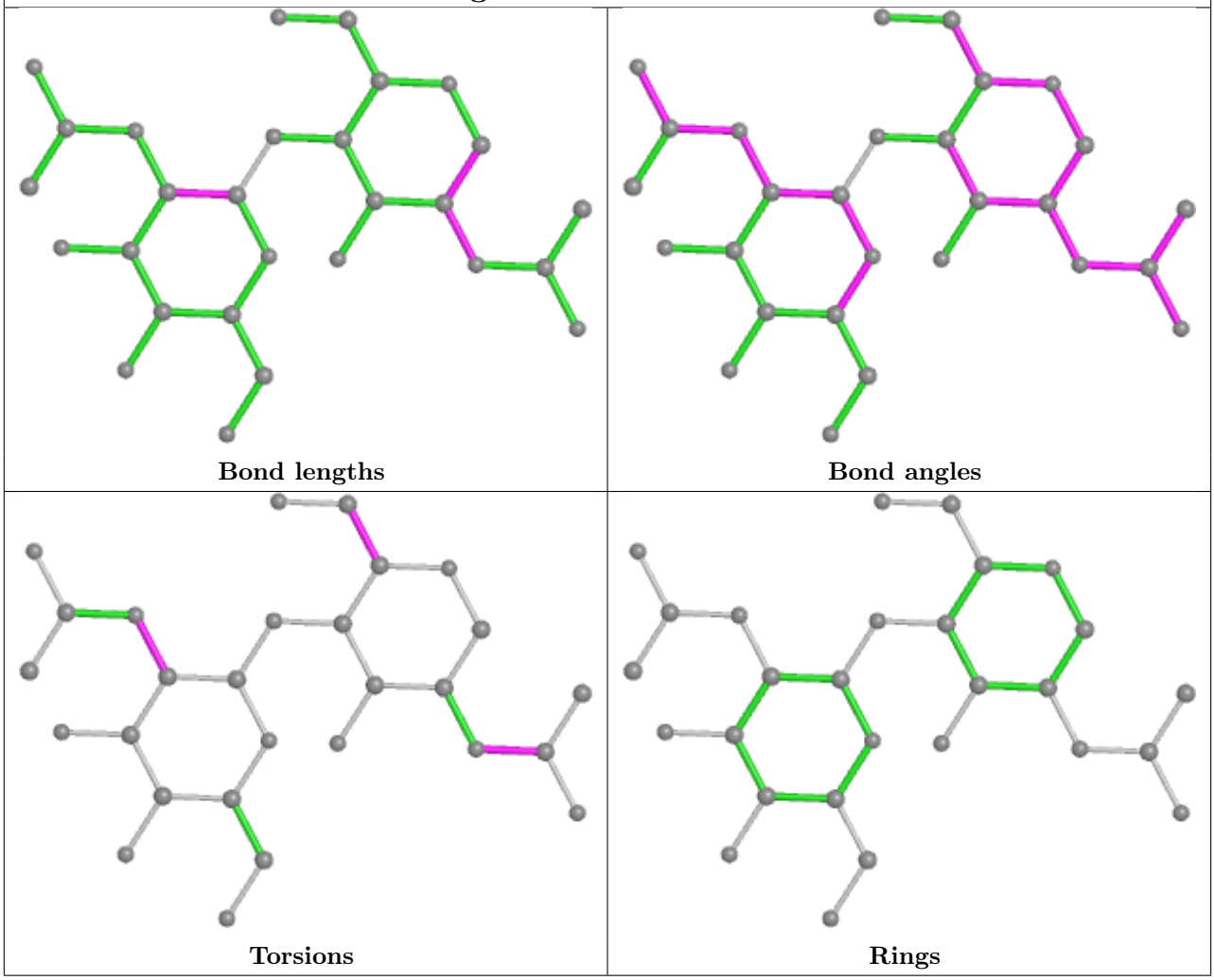


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

1 ligand is 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	CYS	A	395	1	5,6,6	1.53	1 (20%)	5,7,7	2.24	2 (40%)

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	CYS	A	395	1	-	3/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	395	CYS	CB-CA	3.18	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	395	CYS	CB-CA-C	3.51	113.39	109.89
5	A	395	CYS	OXT-C-O	-2.78	117.79	124.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	395	CYS	N-CA-CB-SG
5	A	395	CYS	C-CA-CB-SG
5	A	395	CYS	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	395	CYS	1	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.