Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 08:07 AM EDT

PDB ID	:	1FQ9
Title	:	CRYSTAL STRUCTURE OF A TERNARY FGF2-FGFR1-HEPARIN COMPLEX
Authors	:	Schlessinger, J.; Plotnikov, A.N.; Ibrahimi, O.A.; Eliseenkova, A.V.; Yeh, B.K.; Yayon, A.; Linhardt, R.J.; Mohammadi, M.
Deposited on	:	2000-09-04
Resolution	:	3.00 Å(reported)

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

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

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

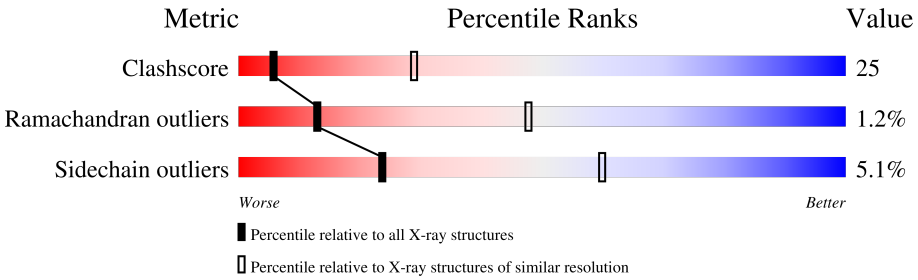
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	132	48% 46%
1	B	132	49% 46%
2	C	225	48% 43% 6%
2	D	225	47% 37% 13%
3	E	8	62% 38%
4	F	6	83% 17%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SGN	E	3	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5496 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 FIBROBLAST GROWTH FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			
1	B	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	CYS	engineered mutation	UNP P09038
A	87	SER	CYS	engineered mutation	UNP P09038
B	69	SER	CYS	engineered mutation	UNP P09038
B	87	SER	CYS	engineered mutation	UNP P09038

- Molecule 2 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1638	1047	280	302	9			
2	D	196	Total	C	N	O	S	0	0	0
			1533	980	263	281	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	ASN	engineered mutation	UNP P11362
D	185	GLN	ASN	engineered mutation	UNP P11362

- Molecule 3 is an oligosaccharide called 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-beta-L-altropyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoami

no)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	S	0	0	0
			140	48	4	76	12			

- Molecule 4 is an oligosaccharide called 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuron ic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-gluc opyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	S	0	0	0
			105	36	3	57	9			

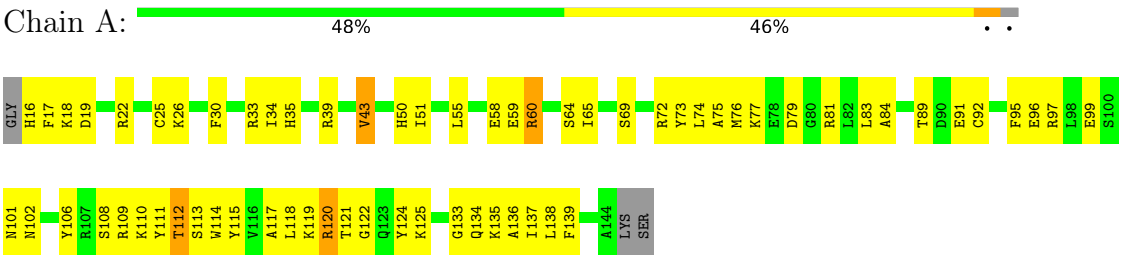
3 Residue-property plots (i)

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.

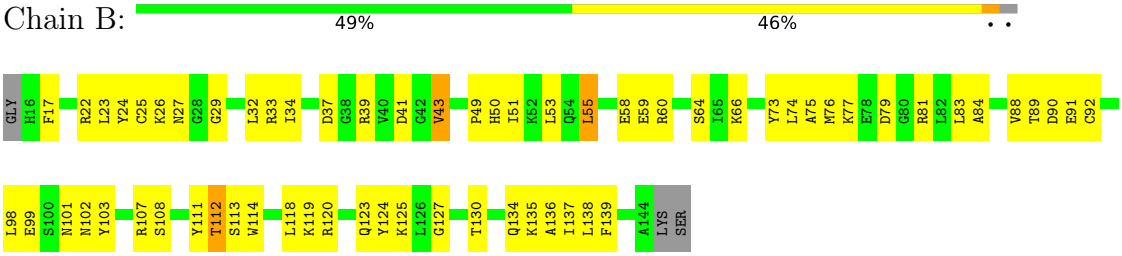
• Molecule 1: FIBROBLAST GROWTH FACTOR 2

Chain A:



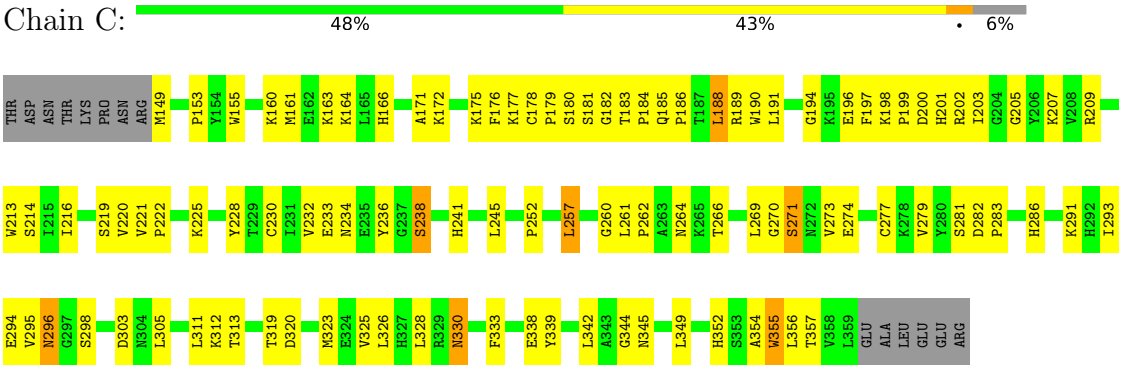
• Molecule 1: FIBROBLAST GROWTH FACTOR 2

Chain B:



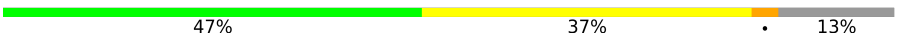
• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1

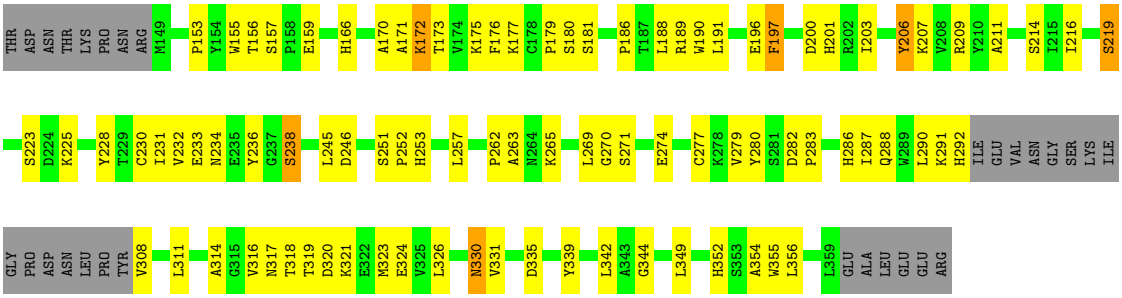
Chain C:



• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1

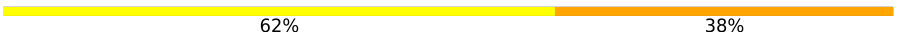
Chain D:





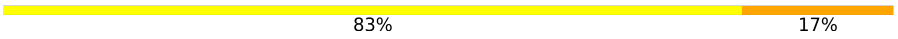
• Molecule 3: 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-beta-L-altropyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain E:



• Molecule 4: 4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.89Å 98.89Å 196.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SGN, IDS, IDU, UAP

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	0.44	0/1063	0.70	1/1425 (0.1%)
1	B	0.45	0/1063	0.68	1/1425 (0.1%)
2	C	0.44	0/1685	0.68	0/2299
2	D	0.42	0/1576	0.69	0/2146
All	All	0.44	0/5387	0.69	2/7295 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	SER	N-CA-C	-5.30	96.68	111.00
1	B	64	SER	N-CA-C	-5.16	97.08	111.00

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	1040	0	1040	59	0
1	B	1040	0	1040	61	0
2	C	1638	0	1603	92	0
2	D	1533	0	1506	82	0
3	E	140	0	44	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	105	0	34	1	0
All	All	5496	0	5267	273	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 25.

All (273) 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)
2:D:175:LYS:HG3	2:D:216:ILE:HG12	1.42	0.99
2:D:282:ASP:HB3	2:D:283:PRO:HD3	1.44	0.98
2:C:282:ASP:HB3	2:C:283:PRO:HD3	1.45	0.96
2:D:286:HIS:HD2	2:D:314:ALA:HB3	1.37	0.90
2:C:207:LYS:HE2	2:C:209:ARG:HE	1.35	0.89
2:C:207:LYS:CE	2:C:209:ARG:HE	1.85	0.88
1:B:88:VAL:HG21	2:D:316:VAL:HG11	1.55	0.88
2:D:286:HIS:CD2	2:D:314:ALA:HB3	2.08	0.88
1:B:76:MET:HE3	1:B:114:TRP:HE3	1.38	0.85
1:A:77:LYS:HD2	1:A:83:LEU:HD21	1.60	0.83
2:C:273:VAL:HG13	2:C:328:LEU:HB2	1.60	0.83
1:B:27:ASN:HA	1:B:135:LYS:HE2	1.60	0.82
1:A:59:GLU:HA	2:C:286:HIS:CD2	2.15	0.81
2:D:344:GLY:HA3	2:D:349:LEU:HD12	1.61	0.81
2:C:344:GLY:HA3	2:C:349:LEU:HD13	1.65	0.78
1:B:76:MET:HE3	1:B:114:TRP:CE3	2.18	0.78
1:A:133:GLY:HA3	2:D:200:ASP:HA	1.66	0.77
2:C:149:MET:O	2:C:149:MET:HG3	1.83	0.77
2:C:164:LYS:HE3	2:C:241:HIS:CE1	2.20	0.77
2:D:171:ALA:O	2:D:219:SER:HA	1.86	0.76
2:D:262:PRO:HG2	2:D:354:ALA:HB2	1.68	0.75
1:A:26:LYS:HD3	1:A:138:LEU:HD12	1.67	0.74
1:B:79:ASP:CG	1:B:81:ARG:HH11	1.91	0.73
2:D:269:LEU:HD23	2:D:270:GLY:N	2.04	0.72
1:B:59:GLU:HA	2:D:286:HIS:ND1	2.04	0.72
1:A:120:ARG:HD3	3:E:4:IDS:O3S	1.92	0.70
2:C:262:PRO:HG2	2:C:354:ALA:HB2	1.73	0.69
1:A:25:CYS:HB2	1:A:139:PHE:CE2	2.28	0.69
2:C:171:ALA:O	2:C:219:SER:HA	1.93	0.69
1:B:119:LYS:HA	4:F:2:IDS:O3S	1.92	0.69
1:B:76:MET:HE1	1:B:114:TRP:HB2	1.75	0.69
2:C:291:LYS:HB2	2:C:311:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:LEU:HD11	2:D:190:TRP:HE1	1.58	0.69
2:C:185:GLN:HE21	2:C:185:GLN:HA	1.59	0.68
2:C:342:LEU:HD11	2:C:349:LEU:HD12	1.75	0.68
1:A:118:LEU:HD23	1:A:124:TYR:HA	1.75	0.67
1:A:97:ARG:HD3	1:A:99:GLU:OE1	1.94	0.67
2:D:209:ARG:CD	2:D:211:ALA:HB3	2.26	0.66
2:D:209:ARG:HE	2:D:211:ALA:H	1.42	0.66
2:D:282:ASP:HB3	2:D:283:PRO:CD	2.23	0.66
1:B:33:ARG:NH1	1:B:43:VAL:HG11	2.11	0.66
2:C:260:GLY:O	2:C:261:LEU:HD23	1.95	0.65
1:A:76:MET:HE3	1:A:114:TRP:HE3	1.61	0.65
2:C:282:ASP:HB3	2:C:283:PRO:CD	2.25	0.65
1:B:55:LEU:N	1:B:55:LEU:HD23	2.11	0.64
1:A:16:HIS:HB3	1:A:19:ASP:OD2	1.96	0.64
2:D:257:LEU:HB2	2:D:352:HIS:CE1	2.32	0.64
1:B:76:MET:CE	1:B:114:TRP:HB2	2.27	0.64
1:B:75:ALA:HB2	1:B:92:CYS:SG	2.38	0.64
1:B:58:GLU:OE1	2:D:316:VAL:HG23	1.98	0.63
1:A:135:LYS:HZ1	2:D:207:LYS:HD3	1.63	0.63
2:D:342:LEU:HD11	2:D:349:LEU:HG	1.79	0.63
2:D:216:ILE:HD13	3:E:8:UAP:H4	1.81	0.63
1:B:79:ASP:OD1	1:B:81:ARG:HD3	1.98	0.63
1:B:119:LYS:HE2	1:B:123:GLN:HB2	1.79	0.63
2:C:296:ASN:C	2:C:298:SER:H	2.01	0.62
1:B:119:LYS:CE	1:B:123:GLN:HB2	2.29	0.62
1:A:135:LYS:NZ	2:D:207:LYS:HD3	2.15	0.62
1:A:16:HIS:CE1	1:A:18:LYS:H	2.17	0.62
2:C:185:GLN:HA	2:C:185:GLN:NE2	2.15	0.61
2:C:222:PRO:O	2:C:225:LYS:HG3	2.00	0.61
1:A:95:PHE:CE1	1:A:109:ARG:HA	2.35	0.61
2:D:209:ARG:HD3	2:D:211:ALA:HB3	1.81	0.61
1:A:60:ARG:NH1	2:C:345:ASN:O	2.33	0.61
1:A:73:TYR:O	1:A:84:ALA:HA	2.01	0.61
2:D:190:TRP:CZ3	2:D:230:CYS:HB3	2.36	0.61
2:C:166:HIS:CD2	2:C:176:PHE:HE1	2.19	0.60
2:D:292:HIS:HD2	2:D:308:VAL:HG12	1.67	0.60
1:B:79:ASP:OD2	1:B:81:ARG:HG2	2.02	0.60
1:B:73:TYR:O	1:B:84:ALA:HA	2.02	0.59
1:B:107:ARG:HD2	1:B:112:THR:O	2.03	0.59
1:A:55:LEU:N	1:A:55:LEU:HD23	2.16	0.59
1:B:66:LYS:HD2	1:B:73:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:HG2	1:A:110:LYS:HD3	1.85	0.59
2:D:291:LYS:HG2	2:D:339:TYR:CE2	2.38	0.59
1:A:96:GLU:HG3	1:A:106:TYR:CE1	2.38	0.58
2:C:160:LYS:HD2	2:C:179:PRO:HG2	1.85	0.58
2:C:185:GLN:HE21	2:C:185:GLN:CA	2.16	0.58
2:D:216:ILE:CD1	3:E:8:UAP:H4	2.34	0.58
1:B:22:ARG:HD3	1:B:51:ILE:HD12	1.86	0.58
2:D:251:SER:HB3	2:D:253:HIS:NE2	2.17	0.58
1:B:24:TYR:CZ	1:B:29:GLY:HA2	2.39	0.57
2:D:157:SER:HB2	2:D:179:PRO:HG3	1.86	0.57
2:C:266:THR:HG23	2:C:357:THR:HG22	1.86	0.57
2:C:163:LYS:HE2	2:C:166:HIS:CE1	2.39	0.57
1:A:101:ASN:O	1:A:102:ASN:HB2	2.03	0.57
2:C:188:LEU:HD12	2:C:213:TRP:HA	1.86	0.57
1:B:119:LYS:HG2	1:B:125:LYS:HZ3	1.70	0.57
2:C:207:LYS:HE2	2:C:209:ARG:HG2	1.87	0.56
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.68	0.56
2:D:159:GLU:HA	2:D:159:GLU:OE1	2.03	0.56
1:A:72:ARG:HD3	1:A:84:ALA:O	2.06	0.56
1:B:101:ASN:O	1:B:102:ASN:HB2	2.06	0.56
2:C:221:VAL:HB	2:C:222:PRO:HD2	1.86	0.56
2:C:338:GLU:HB2	2:C:355:TRP:CE2	2.41	0.56
2:C:293:ILE:HG22	2:C:294:GLU:N	2.22	0.54
2:D:172:LYS:HD3	2:D:173:THR:O	2.07	0.54
2:D:233:GLU:HB3	2:D:238:SER:HB2	1.89	0.54
2:D:155:TRP:CE3	2:D:180:SER:HB3	2.43	0.54
1:A:59:GLU:CA	2:C:286:HIS:CD2	2.90	0.53
2:C:191:LEU:HD13	2:C:194:GLY:O	2.07	0.53
1:B:60:ARG:HD2	2:D:349:LEU:HD13	1.89	0.53
2:D:186:PRO:HB2	2:D:232:VAL:HG12	1.89	0.53
1:A:97:ARG:HD3	1:A:99:GLU:CD	2.29	0.53
2:C:257:LEU:HD22	2:C:279:VAL:HG22	1.92	0.52
2:C:257:LEU:HB2	2:C:352:HIS:CE1	2.45	0.52
2:D:318:THR:CG2	2:D:323:MET:SD	2.98	0.52
2:C:303:ASP:CG	2:C:305:LEU:HD23	2.30	0.52
2:C:207:LYS:HE2	2:C:209:ARG:NE	2.16	0.52
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.25	0.52
2:D:180:SER:OG	2:D:232:VAL:HG11	2.10	0.52
2:D:190:TRP:CH2	2:D:230:CYS:HB3	2.45	0.52
1:B:49:PRO:HG2	1:B:50:HIS:CD2	2.45	0.52
2:C:155:TRP:CE3	2:C:180:SER:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:LYS:HB3	2:C:214:SER:OG	2.09	0.52
2:D:291:LYS:HB2	2:D:311:LEU:HD11	1.92	0.51
1:A:58:GLU:O	1:A:59:GLU:HB3	2.10	0.51
1:A:79:ASP:CG	1:A:81:ARG:HH11	2.13	0.51
1:A:125:LYS:NZ	1:A:134:GLN:NE2	2.58	0.51
2:C:257:LEU:HD13	2:C:277:CYS:SG	2.49	0.51
2:C:295:VAL:HG12	2:C:295:VAL:O	2.10	0.51
1:B:79:ASP:OD2	1:B:81:ARG:NH1	2.41	0.51
2:C:153:PRO:HG3	2:C:233:GLU:HA	1.91	0.51
1:A:111:TYR:O	1:A:113:SER:N	2.43	0.51
1:A:16:HIS:CE1	1:A:18:LYS:CB	2.93	0.51
2:C:153:PRO:HA	2:C:181:SER:O	2.10	0.51
2:C:236:TYR:N	2:C:236:TYR:CD1	2.79	0.51
2:D:157:SER:HB2	2:D:179:PRO:CG	2.40	0.51
1:A:115:TYR:HB2	1:A:137:ILE:HG22	1.93	0.51
2:C:260:GLY:C	2:C:261:LEU:HD23	2.31	0.51
2:C:264:ASN:OD1	2:C:355:TRP:N	2.30	0.51
1:A:95:PHE:CZ	1:A:109:ARG:HG3	2.46	0.51
2:C:296:ASN:C	2:C:298:SER:N	2.64	0.51
2:D:236:TYR:N	2:D:236:TYR:CD1	2.78	0.51
2:D:153:PRO:HA	2:D:181:SER:O	2.11	0.51
2:D:170:ALA:O	2:D:171:ALA:HB3	2.10	0.51
2:D:207:LYS:NZ	3:E:7:SGN:H3	2.26	0.50
1:B:59:GLU:HA	2:D:286:HIS:CG	2.46	0.50
1:B:17:PHE:HE1	2:D:320:ASP:HB3	1.77	0.50
2:C:172:LYS:O	2:C:220:VAL:HG22	2.11	0.49
1:A:125:LYS:HZ2	1:A:134:GLN:NE2	2.10	0.49
2:C:262:PRO:HD2	2:C:352:HIS:HB3	1.94	0.49
1:A:30:PHE:CD2	1:A:122:GLY:HA2	2.48	0.49
1:B:26:LYS:O	1:B:135:LYS:HE2	2.11	0.49
1:B:118:LEU:HD23	1:B:124:TYR:HA	1.94	0.49
2:C:295:VAL:O	2:C:296:ASN:CG	2.51	0.49
2:D:262:PRO:HD2	2:D:352:HIS:HB3	1.93	0.49
2:C:175:LYS:HG3	2:C:216:ILE:HD13	1.93	0.49
2:D:188:LEU:HD23	2:D:232:VAL:HG22	1.95	0.49
1:A:120:ARG:HD3	1:A:120:ARG:H	1.77	0.48
1:B:33:ARG:NH2	1:B:43:VAL:HG13	2.28	0.48
1:B:83:LEU:C	1:B:83:LEU:HD12	2.34	0.48
2:C:269:LEU:HD12	2:C:333:PHE:CD2	2.49	0.48
1:A:60:ARG:HD2	2:C:349:LEU:HD11	1.94	0.48
1:B:111:TYR:O	1:B:113:SER:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH1	1:B:43:VAL:CG1	2.76	0.48
1:A:76:MET:HE1	1:A:114:TRP:HB2	1.96	0.48
2:C:266:THR:HG23	2:C:357:THR:CG2	2.44	0.48
1:A:33:ARG:NH1	1:A:43:VAL:HG11	2.29	0.47
1:B:134:GLN:O	1:B:137:ILE:HG12	2.14	0.47
1:A:22:ARG:HD3	1:A:51:ILE:HD12	1.95	0.47
1:B:25:CYS:HB2	1:B:139:PHE:CE2	2.50	0.47
2:D:245:LEU:HD12	2:D:246:ASP:N	2.29	0.47
2:C:291:LYS:HD3	2:C:339:TYR:CZ	2.50	0.47
1:B:37:ASP:OD1	1:B:39:ARG:HG3	2.15	0.47
2:D:188:LEU:HD11	2:D:190:TRP:NE1	2.26	0.47
1:A:83:LEU:HD12	1:A:83:LEU:C	2.36	0.46
2:D:271:SER:O	2:D:330:ASN:HA	2.14	0.46
1:A:33:ARG:CZ	1:A:43:VAL:HG13	2.45	0.46
1:B:33:ARG:HG3	1:B:50:HIS:O	2.15	0.46
1:B:26:LYS:HB2	1:B:103:TYR:CE1	2.50	0.46
2:C:191:LEU:O	2:C:228:TYR:HA	2.16	0.46
2:D:191:LEU:HD23	2:D:196:GLU:HA	1.97	0.46
2:C:153:PRO:HD3	2:C:234:ASN:CG	2.35	0.46
2:C:271:SER:O	2:C:330:ASN:HA	2.16	0.46
1:A:76:MET:O	1:A:111:TYR:HE2	1.99	0.46
1:A:115:TYR:HB2	1:A:137:ILE:CG2	2.46	0.46
2:C:186:PRO:HG2	2:C:213:TRP:CH2	2.51	0.46
2:D:153:PRO:HG3	2:D:233:GLU:HA	1.98	0.46
1:B:27:ASN:ND2	1:B:120:ARG:N	2.63	0.46
1:A:16:HIS:ND1	1:A:17:PHE:N	2.64	0.45
1:B:77:LYS:HA	1:B:91:GLU:OE2	2.15	0.45
2:C:221:VAL:HB	2:C:222:PRO:CD	2.45	0.45
2:D:318:THR:HG21	2:D:323:MET:SD	2.57	0.45
1:A:65:ILE:HD12	1:A:74:LEU:HD23	1.97	0.45
1:B:23:LEU:HG	1:B:53:LEU:HD12	1.97	0.45
2:C:274:GLU:HA	2:C:326:LEU:O	2.17	0.45
2:D:245:LEU:HD12	2:D:246:ASP:H	1.82	0.45
1:A:60:ARG:CZ	2:C:349:LEU:HD21	2.47	0.45
2:D:189:ARG:HD3	2:D:233:GLU:OE1	2.17	0.45
1:B:98:LEU:HD21	2:D:252:PRO:HB3	1.99	0.45
2:C:198:LYS:N	2:C:201:HIS:CD2	2.85	0.45
2:D:189:ARG:HG3	2:D:231:ILE:HB	1.99	0.45
2:D:277:CYS:O	2:D:324:GLU:HG2	2.17	0.45
1:B:32:LEU:HD21	1:B:74:LEU:HD22	1.98	0.45
2:C:188:LEU:HD23	2:C:189:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:THR:HG22	2:D:318:THR:O	2.15	0.45
2:C:319:THR:HG22	2:C:320:ASP:N	2.31	0.45
2:C:213:TRP:CZ3	2:C:232:VAL:HG13	2.52	0.45
1:A:117:ALA:HB1	1:A:136:ALA:HB1	1.99	0.44
2:C:257:LEU:N	2:C:257:LEU:HD23	2.32	0.44
1:A:60:ARG:NE	2:C:349:LEU:HD21	2.33	0.44
1:B:34:ILE:O	1:B:50:HIS:HB3	2.18	0.44
1:B:127:GLY:HA2	1:B:130:THR:HG23	1.98	0.44
2:C:196:GLU:OE1	2:C:198:LYS:HE3	2.17	0.44
2:D:263:ALA:O	2:D:265:LYS:HG3	2.18	0.44
2:C:270:GLY:O	2:C:330:ASN:HA	2.18	0.44
2:D:191:LEU:O	2:D:228:TYR:HA	2.16	0.44
2:D:319:THR:HG21	2:D:321:LYS:NZ	2.33	0.44
2:C:293:ILE:HG22	2:C:294:GLU:H	1.82	0.44
1:B:33:ARG:CZ	1:B:43:VAL:HG13	2.47	0.44
1:B:33:ARG:HH21	1:B:41:ASP:CG	2.20	0.44
2:C:180:SER:OG	2:C:232:VAL:HG11	2.17	0.44
2:D:331:VAL:HA	2:D:335:ASP:OD2	2.18	0.44
2:C:186:PRO:HB2	2:C:232:VAL:HG12	2.00	0.43
2:D:270:GLY:O	2:D:330:ASN:HA	2.18	0.43
1:B:88:VAL:HG21	2:D:316:VAL:CG1	2.36	0.43
2:C:261:LEU:HA	2:C:262:PRO:C	2.39	0.43
2:D:156:THR:HG23	2:D:180:SER:HA	2.00	0.43
2:D:291:LYS:HE3	2:D:339:TYR:CE1	2.53	0.43
2:C:233:GLU:HB3	2:C:238:SER:HB2	2.01	0.43
2:C:338:GLU:HB2	2:C:355:TRP:CZ2	2.53	0.43
1:B:99:GLU:HB2	1:B:101:ASN:OD1	2.18	0.43
2:C:190:TRP:CZ3	2:C:230:CYS:HB3	2.53	0.43
2:C:202:ARG:HG2	2:C:205:GLY:HA2	2.01	0.43
1:B:99:GLU:HB3	2:C:203:ILE:HG12	2.01	0.43
2:C:161:MET:CE	2:C:178:CYS:HA	2.49	0.43
2:C:171:ALA:HA	2:C:219:SER:HA	2.01	0.43
1:A:26:LYS:CD	1:A:138:LEU:HD12	2.43	0.42
2:C:188:LEU:CD1	2:C:213:TRP:HA	2.49	0.42
2:D:166:HIS:CG	2:D:176:PHE:HE1	2.37	0.42
1:A:76:MET:CE	1:A:114:TRP:HB2	2.49	0.42
1:B:125:LYS:HE2	1:B:136:ALA:CB	2.49	0.42
2:D:234:ASN:C	2:D:234:ASN:OD1	2.58	0.42
1:A:77:LYS:HE2	1:A:77:LYS:HA	2.01	0.42
1:A:119:LYS:C	1:A:121:THR:H	2.23	0.42
1:B:26:LYS:HD3	1:B:138:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:TRP:HE3	2:D:180:SER:HB3	1.82	0.42
1:A:75:ALA:HB2	1:A:92:CYS:SG	2.59	0.42
2:C:325:VAL:O	2:C:325:VAL:HG13	2.20	0.42
1:B:27:ASN:HB2	1:B:136:ALA:HA	2.02	0.42
1:A:60:ARG:HD2	2:C:349:LEU:CD1	2.49	0.42
1:A:35:HIS:CD2	1:A:39:ARG:HB2	2.54	0.41
2:C:303:ASP:O	2:C:305:LEU:HD22	2.20	0.41
2:D:257:LEU:CD2	2:D:279:VAL:HG22	2.50	0.41
2:D:279:VAL:HG12	2:D:280:TYR:N	2.35	0.41
2:D:288:GLN:HG2	2:D:290:LEU:CD1	2.50	0.41
1:B:125:LYS:HZ3	1:B:125:LYS:HB2	1.86	0.41
1:A:22:ARG:HD3	1:A:51:ILE:CD1	2.51	0.41
1:B:33:ARG:NH2	1:B:41:ASP:OD1	2.53	0.41
1:B:60:ARG:HH11	2:D:349:LEU:HD13	1.85	0.41
1:B:81:ARG:HB2	1:B:124:TYR:OH	2.21	0.41
2:C:166:HIS:O	2:C:245:LEU:HD12	2.21	0.41
2:C:186:PRO:HG2	2:C:213:TRP:HH2	1.86	0.41
2:C:190:TRP:CH2	2:C:230:CYS:HB3	2.55	0.41
2:C:198:LYS:H	2:C:201:HIS:CD2	2.39	0.41
2:C:203:ILE:C	2:C:205:GLY:H	2.24	0.41
2:D:225:LYS:HE2	2:D:246:ASP:OD2	2.21	0.41
1:A:34:ILE:O	1:A:50:HIS:HB3	2.20	0.41
1:B:88:VAL:CG2	2:D:316:VAL:HG11	2.39	0.41
2:C:312:LYS:HG2	2:C:323:MET:SD	2.61	0.41
2:D:269:LEU:HD23	2:D:269:LEU:C	2.39	0.41
2:C:182:GLY:O	2:C:186:PRO:HD3	2.21	0.40
2:D:177:LYS:HB3	2:D:214:SER:HB3	2.03	0.40
1:B:108:SER:O	1:B:112:THR:HA	2.20	0.40
2:D:153:PRO:HB3	2:D:186:PRO:HB3	2.03	0.40
1:A:81:ARG:HB2	1:A:124:TYR:OH	2.21	0.40
2:D:274:GLU:HA	2:D:326:LEU:O	2.22	0.40
2:D:287:ILE:HG22	2:D:288:GLN:N	2.36	0.40
1:A:108:SER:O	1:A:112:THR:HA	2.21	0.40
2:D:197:PHE:HD1	2:D:206:TYR:CZ	2.39	0.40
2:C:161:MET:HE3	2:C:178:CYS:HA	2.04	0.40
2:C:183:THR:HA	2:C:184:PRO:C	2.41	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	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	19 57
1	B	127/132 (96%)	116 (91%)	10 (8%)	1 (1%)	19 57
2	C	209/225 (93%)	194 (93%)	11 (5%)	4 (2%)	8 36
2	D	192/225 (85%)	176 (92%)	14 (7%)	2 (1%)	15 53
All	All	655/714 (92%)	602 (92%)	45 (7%)	8 (1%)	13 48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	B	112	THR
2	C	271	SER
2	C	296	ASN
2	C	281	SER
2	D	219	SER
2	D	330	ASN
2	C	330	ASN

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	110/113 (97%)	105 (96%)	5 (4%)	27 64
1	B	110/113 (97%)	106 (96%)	4 (4%)	35 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	180/198 (91%)	170 (94%)	10 (6%)	21 56
2	D	169/198 (85%)	159 (94%)	10 (6%)	19 54
All	All	569/622 (92%)	540 (95%)	29 (5%)	24 60

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	60	ARG
1	A	69	SER
1	A	89	THR
1	A	120	ARG
1	B	43	VAL
1	B	55	LEU
1	B	89	THR
1	B	90	ASP
2	C	188	LEU
2	C	197	PHE
2	C	199	PRO
2	C	200	ASP
2	C	238	SER
2	C	252	PRO
2	C	257	LEU
2	C	313	THR
2	C	355	TRP
2	C	356	LEU
2	D	172	LYS
2	D	197	PHE
2	D	201	HIS
2	D	203	ILE
2	D	206	TYR
2	D	223	SER
2	D	238	SER
2	D	317	ASN
2	D	355	TRP
2	D	356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	134	GLN
1	B	27	ASN
2	C	166	HIS
2	C	185	GLN
2	C	201	HIS
2	C	286	HIS
2	C	317	ASN
2	C	330	ASN
2	D	292	HIS
2	D	317	ASN

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)

14 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	SGN	E	1	3	19,20,20	4.01	3 (15%)	24,31,31	1.39	3 (12%)
3	IDU	E	2	3	13,16,17	2.33	3 (23%)	15,24,26	1.51	1 (6%)
3	SGN	E	3	3	18,19,20	3.73	4 (22%)	22,29,31	1.64	3 (13%)
3	IDS	E	4	3	13,16,17	2.38	5 (38%)	15,24,26	1.74	4 (26%)
3	SGN	E	5	3	18,19,20	3.40	3 (16%)	22,29,31	1.56	5 (22%)
3	IDS	E	6	3	13,16,17	2.55	3 (23%)	15,24,26	2.09	5 (33%)
3	SGN	E	7	3	18,19,20	3.26	4 (22%)	22,29,31	2.14	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	UAP	E	8	3	12,15,16	5.68	6 (50%)	13,22,24	3.38	4 (30%)
4	SGN	F	1	4	19,20,20	3.41	3 (15%)	24,31,31	1.31	2 (8%)
4	IDS	F	2	4	13,16,17	2.46	5 (38%)	15,24,26	2.88	4 (26%)
4	SGN	F	3	4	18,19,20	3.46	2 (11%)	22,29,31	1.58	3 (13%)
4	IDS	F	4	4	13,16,17	2.43	2 (15%)	15,24,26	1.75	4 (26%)
4	SGN	F	5	4	18,19,20	3.66	3 (16%)	22,29,31	1.63	5 (22%)
4	UAP	F	6	4	12,15,16	5.88	5 (41%)	13,22,24	3.51	5 (38%)

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	SGN	E	1	3	-	4/11/31/31	0/1/1/1
3	IDU	E	2	3	-	3/5/26/29	0/1/1/1
3	SGN	E	3	3	1/1/6/8	5/11/28/31	0/1/1/1
3	IDS	E	4	3	-	3/5/26/29	0/1/1/1
3	SGN	E	5	3	-	6/11/28/31	0/1/1/1
3	IDS	E	6	3	-	3/5/26/29	0/1/1/1
3	SGN	E	7	3	-	2/11/28/31	0/1/1/1
3	UAP	E	8	3	-	0/5/22/25	0/1/1/1
4	SGN	F	1	4	-	3/11/31/31	0/1/1/1
4	IDS	F	2	4	-	1/5/26/29	0/1/1/1
4	SGN	F	3	4	-	0/11/28/31	0/1/1/1
4	IDS	F	4	4	-	0/5/26/29	0/1/1/1
4	SGN	F	5	4	-	8/11/28/31	0/1/1/1
4	UAP	F	6	4	-	3/5/22/25	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6	UAP	C4-C5	17.72	1.53	1.32
3	E	8	UAP	C4-C5	17.07	1.52	1.32
3	E	1	SGN	S1-N2	14.64	1.79	1.59
4	F	5	SGN	S1-N2	13.17	1.77	1.59
3	E	3	SGN	S1-N2	12.90	1.76	1.59
4	F	3	SGN	S1-N2	12.46	1.76	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	SGN	S1-N2	12.40	1.76	1.59
3	E	5	SGN	S1-N2	12.09	1.75	1.59
3	E	7	SGN	S1-N2	11.13	1.74	1.59
3	E	1	SGN	O6-S2	8.34	1.79	1.56
3	E	3	SGN	O6-S2	8.11	1.78	1.56
3	E	5	SGN	O6-S2	7.11	1.76	1.56
4	F	5	SGN	O6-S2	7.07	1.76	1.56
4	F	1	SGN	O6-S2	7.05	1.76	1.56
3	E	7	SGN	O6-S2	7.02	1.76	1.56
4	F	2	IDS	O2-S	6.87	1.77	1.57
4	F	3	SGN	O6-S2	6.76	1.75	1.56
3	E	2	IDU	O2-S	6.63	1.76	1.57
4	F	4	IDS	O2-S	6.25	1.75	1.57
3	E	6	IDS	O2-S	6.22	1.75	1.57
3	E	8	UAP	O2-S	6.20	1.75	1.57
4	F	6	UAP	O2-S	5.85	1.74	1.57
3	E	4	IDS	O2-S	5.64	1.73	1.57
3	E	6	IDS	O2-C2	-5.52	1.38	1.47
4	F	6	UAP	O2-C2	-5.22	1.39	1.47
4	F	4	IDS	O2-C2	-4.97	1.39	1.47
3	E	8	UAP	O2-C2	-4.80	1.39	1.47
3	E	4	IDS	O2-C2	-4.66	1.40	1.47
4	F	6	UAP	C3-C4	4.24	1.55	1.50
3	E	2	IDU	O2-C2	-3.81	1.41	1.47
3	E	8	UAP	C3-C4	3.80	1.55	1.50
4	F	6	UAP	O5-C5	3.39	1.42	1.37
4	F	2	IDS	O2-C2	-3.06	1.42	1.47
3	E	8	UAP	O5-C5	2.96	1.41	1.37
3	E	3	SGN	O1S-S1	2.75	1.45	1.42
3	E	8	UAP	O3-C3	-2.57	1.38	1.43
4	F	2	IDS	O5-C5	-2.49	1.41	1.43
3	E	4	IDS	O3-C3	-2.48	1.37	1.43
4	F	2	IDS	C1-C2	2.46	1.55	1.51
3	E	1	SGN	O1S-S1	2.44	1.44	1.42
3	E	4	IDS	O5-C5	-2.40	1.41	1.43
3	E	7	SGN	C2-N2	-2.38	1.43	1.47
3	E	6	IDS	O5-C5	-2.38	1.41	1.43
3	E	5	SGN	C2-N2	-2.34	1.43	1.47
3	E	2	IDU	C1-C2	2.34	1.55	1.51
4	F	2	IDS	O3-C3	-2.26	1.37	1.43
3	E	7	SGN	O1S-S1	2.21	1.44	1.42
4	F	5	SGN	O1S-S1	2.18	1.44	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	SGN	O1S-S1	2.14	1.44	1.42
3	E	3	SGN	C2-N2	-2.13	1.44	1.47
3	E	4	IDS	C1-C2	2.01	1.54	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6	UAP	C1-C2-C3	10.40	118.60	108.98
3	E	8	UAP	C1-C2-C3	9.79	118.04	108.98
4	F	2	IDS	C1-C2-C3	8.23	121.70	109.40
3	E	7	SGN	C3-C2-N2	-6.83	101.35	110.32
3	E	6	IDS	C1-C2-C3	5.17	117.12	109.40
4	F	2	IDS	O2-C2-C3	5.13	114.12	106.95
4	F	6	UAP	C3-C4-C5	-4.72	113.61	121.60
3	E	3	SGN	C3-C2-N2	-4.59	104.29	110.32
3	E	8	UAP	C3-C4-C5	-4.51	113.98	121.60
3	E	5	SGN	O2S-S1-O1S	-4.43	109.68	120.16
4	F	2	IDS	C1-O5-C5	4.32	119.78	112.17
3	E	2	IDU	C1-O5-C5	4.31	119.77	112.17
3	E	1	SGN	O2S-S1-O1S	-4.08	110.52	120.16
4	F	3	SGN	O2S-S1-O1S	-4.08	110.52	120.16
4	F	1	SGN	O2S-S1-O1S	-4.07	110.55	120.16
4	F	4	IDS	C1-C2-C3	4.05	115.46	109.40
3	E	8	UAP	C2-O2-S	-4.03	112.65	117.91
4	F	5	SGN	O2S-S1-O1S	-3.99	110.72	120.16
3	E	3	SGN	O2S-S1-O1S	-3.96	110.81	120.16
4	F	3	SGN	C3-C2-N2	-3.94	105.14	110.32
3	E	7	SGN	O2S-S1-O1S	-3.93	110.87	120.16
4	F	4	IDS	C1-O5-C5	3.84	118.94	112.17
3	E	4	IDS	C1-C2-C3	3.66	114.87	109.40
3	E	4	IDS	C2-O2-S	-3.58	113.24	117.91
4	F	6	UAP	C2-O2-S	-3.44	113.43	117.91
3	E	6	IDS	C2-O2-S	-3.42	113.45	117.91
3	E	6	IDS	C1-O5-C5	3.40	118.17	112.17
3	E	1	SGN	C4-C3-C2	-3.29	105.53	110.34
4	F	5	SGN	C3-C2-N2	-3.23	106.08	110.32
3	E	7	SGN	C1-C2-N2	-3.14	104.87	110.27
3	E	7	SGN	C1-O5-C5	3.03	116.30	112.19
4	F	1	SGN	C1-C2-N2	-2.99	107.10	110.67
3	E	5	SGN	C3-C2-N2	-2.86	106.56	110.32
4	F	5	SGN	C4-C3-C2	-2.82	106.89	111.02
3	E	8	UAP	C2-C3-C4	2.82	115.21	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6	UAP	C2-C3-C4	2.78	115.14	109.77
3	E	4	IDS	C1-O5-C5	2.53	116.63	112.17
3	E	6	IDS	O4-C4-C5	-2.51	105.26	110.05
4	F	4	IDS	C2-O2-S	-2.46	114.71	117.91
3	E	7	SGN	C3-C4-C5	-2.43	105.90	110.24
4	F	2	IDS	C4-C3-C2	2.37	114.46	110.24
3	E	6	IDS	O2-C2-C3	2.37	110.25	106.95
3	E	5	SGN	C1-C2-N2	-2.28	106.35	110.27
3	E	4	IDS	O2-C2-C3	2.28	110.14	106.95
3	E	5	SGN	C4-C3-C2	-2.26	107.71	111.02
3	E	3	SGN	C1-O5-C5	-2.25	109.15	112.19
4	F	4	IDS	O4-C4-C5	-2.23	105.80	110.05
3	E	7	SGN	O6-C6-C5	2.11	111.56	107.62
3	E	1	SGN	C1-C2-C3	2.10	113.41	110.54
4	F	5	SGN	C1-C2-N2	-2.09	106.68	110.27
4	F	3	SGN	C1-O5-C5	2.08	115.02	112.19
3	E	5	SGN	C1-O5-C5	2.07	115.00	112.19
4	F	5	SGN	O6-C6-C5	2.04	111.43	107.62
4	F	6	UAP	C1-O5-C5	2.02	119.82	115.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	3	SGN	C1

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	IDU	C2-O2-S-O1S
3	E	2	IDU	C2-O2-S-O2S
3	E	2	IDU	C2-O2-S-O3S
3	E	3	SGN	O5-C5-C6-O6
3	E	3	SGN	C2-N2-S1-O3S
3	E	3	SGN	C6-O6-S2-O5S
3	E	4	IDS	C2-O2-S-O3S
3	E	5	SGN	O5-C5-C6-O6
3	E	5	SGN	C6-O6-S2-O6S
3	E	6	IDS	C2-O2-S-O1S
3	E	6	IDS	C2-O2-S-O3S
3	E	7	SGN	C4-C5-C6-O6
3	E	7	SGN	O5-C5-C6-O6
4	F	1	SGN	C4-C5-C6-O6

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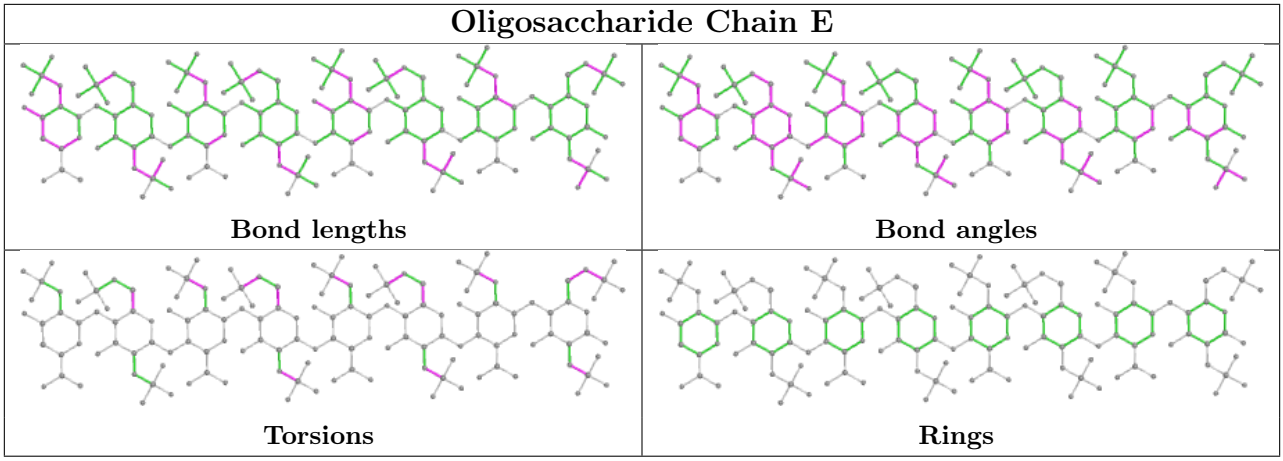
Mol	Chain	Res	Type	Atoms
4	F	1	SGN	O5-C5-C6-O6
4	F	2	IDS	C1-C2-O2-S
4	F	5	SGN	C4-C5-C6-O6
4	F	5	SGN	O5-C5-C6-O6
4	F	5	SGN	C2-N2-S1-O1S
4	F	5	SGN	C2-N2-S1-O3S
3	E	5	SGN	C6-O6-S2-O4S
3	E	5	SGN	C6-O6-S2-O5S
3	E	3	SGN	C6-O6-S2-O6S
4	F	5	SGN	C6-O6-S2-O6S
3	E	4	IDS	C2-O2-S-O1S
3	E	4	IDS	C2-O2-S-O2S
3	E	6	IDS	C2-O2-S-O2S
4	F	6	UAP	C2-O2-S-O2S
4	F	5	SGN	C6-O6-S2-O5S
3	E	3	SGN	C6-O6-S2-O4S
4	F	5	SGN	C6-O6-S2-O4S
3	E	5	SGN	C4-C5-C6-O6
4	F	6	UAP	C2-O2-S-O1S
4	F	6	UAP	C2-O2-S-O3S
3	E	1	SGN	C6-O6-S2-O5S
3	E	1	SGN	C2-N2-S1-O1S
3	E	5	SGN	C2-N2-S1-O1S
4	F	5	SGN	C2-N2-S1-O2S
3	E	1	SGN	C6-O6-S2-O4S
3	E	1	SGN	C5-C6-O6-S2
4	F	1	SGN	C2-N2-S1-O2S

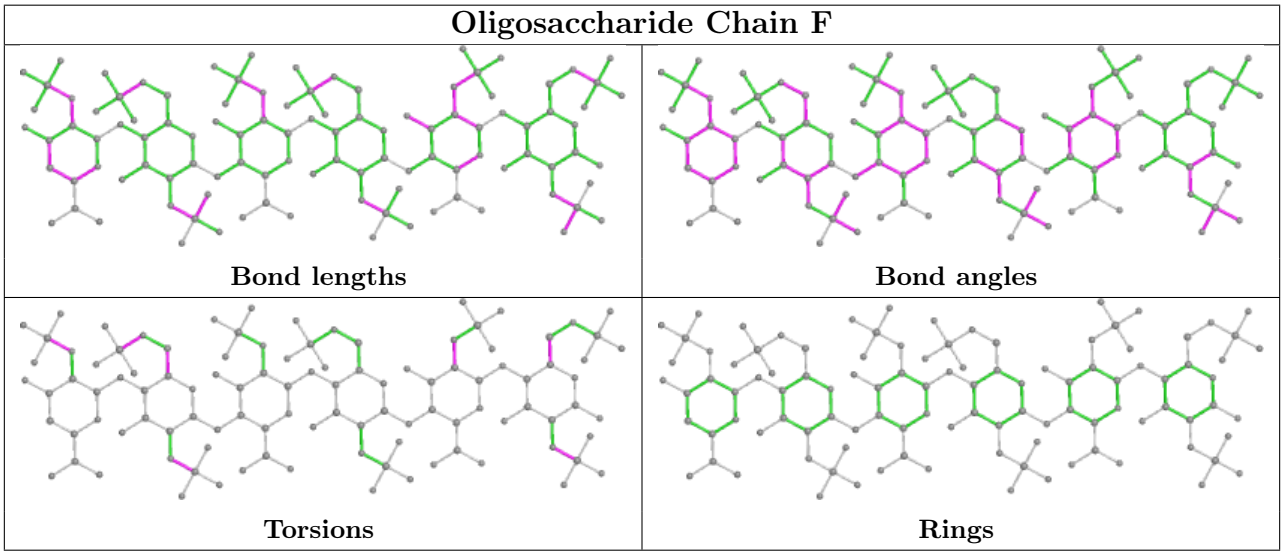
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7	SGN	1	0
3	E	4	IDS	1	0
4	F	2	IDS	1	0
3	E	8	UAP	2	0

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





5.6 Ligand geometry

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.