Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:01 PM EDT

PDB ID	:	1E0O
Title	:	CRYSTAL STRUCTURE OF A TERNARY FGF1-FGFR2-HEPARIN COMPLEX
Authors	:	Pellegrini, L.; Burke, D.F.; von Delft, F.; Mulloy, B.; Blundell, T.L.
Deposited on	:	2000-04-03
Resolution	:	2.80 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:

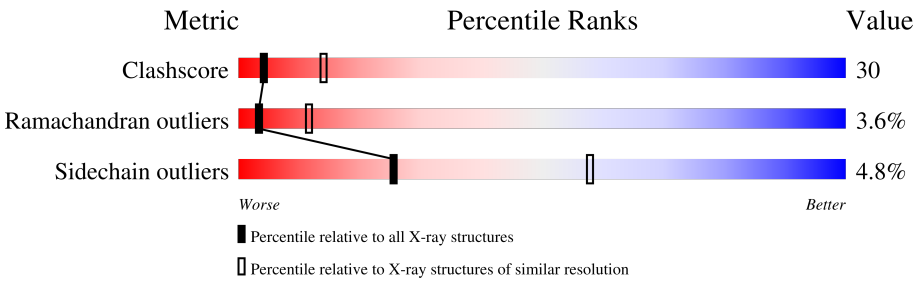
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	140	38% 47% 7% 8%
1	C	140	46% 41% 5% 7%
2	B	219	51% 36% • 10%
2	D	219	47% 39% • 11%
3	E	10	60% 40%

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	SO4	D	401	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5247 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.

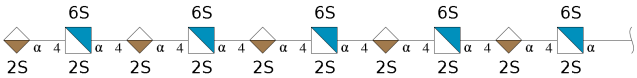
- Molecule 1 is a protein called FIBROBLAST GROWTH FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	979	622	173	180	4	0	0	0
1	C	130	1017	642	178	193	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	197	1505	955	266	276	8	0	0	0
2	D	196	1500	950	266	276	8	0	0	0

- Molecule 3 is an oligosaccharide called 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-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-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.

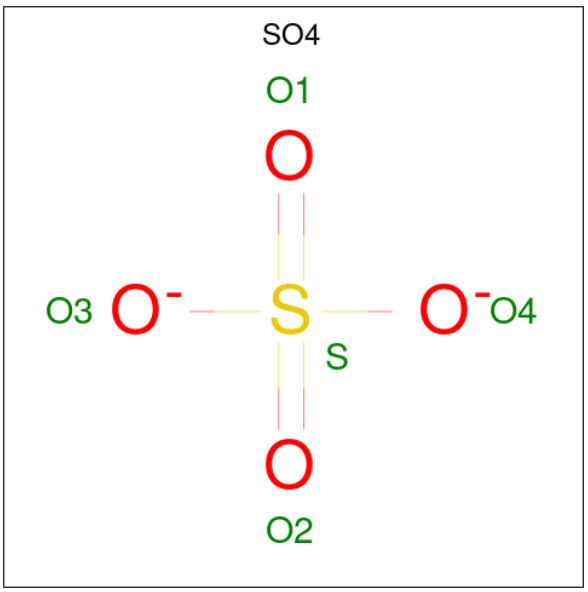


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	10	175	60	5	95	15	0	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0
4	B	2	Total Ni 2 2	0	0
4	C	1	Total Ni 1 1	0	0
4	D	1	Total Ni 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	12	12	12	0	0
			Total	O		
6	C	7	7	7	0	0
			Total	O		
6	D	15	15	15	0	0

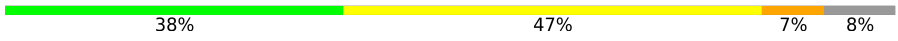
3 Residue-property plots (i)

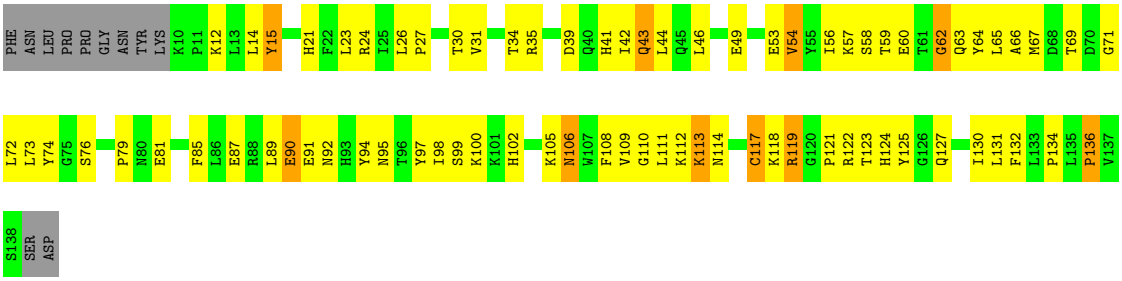
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: FIBROBLAST GROWTH FACTOR 1

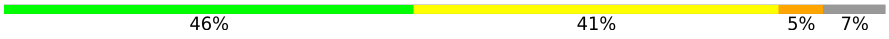
Chain A:

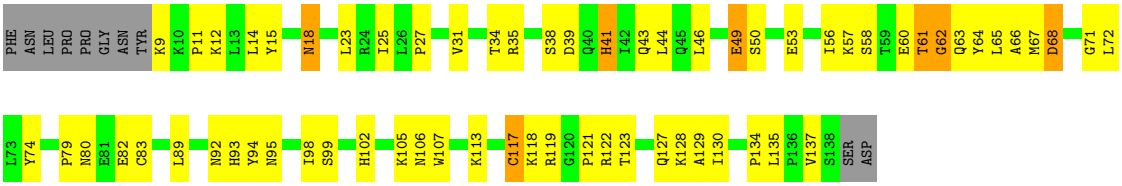




• Molecule 1: FIBROBLAST GROWTH FACTOR 1

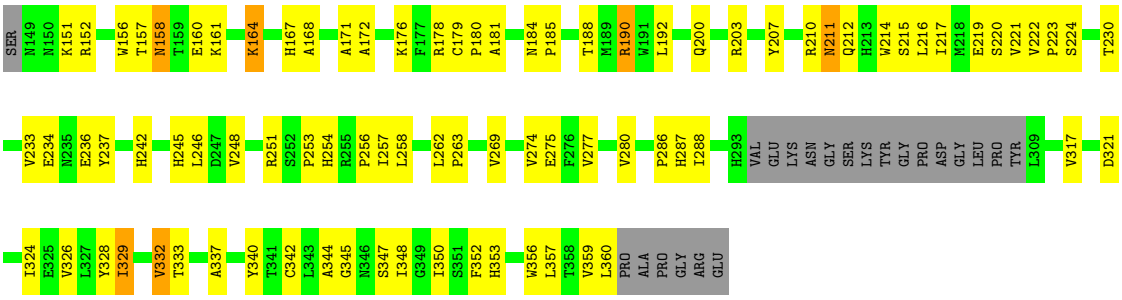
Chain C:





• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 2

Chain B:



• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 2

Chain D: 47% 39% • 11%

SER N149 R152 A153 P154 Y155 N158 T159 E163 H167 A168 V169 P170 A171 A172 N173 T174 V175 K176 F177 P180 A181 G182 G183 N184 P185 M186 P187 W191 L192 K193 N194 E197 F198 K199 H202 R203 I204 G205 G206 Y207 R210 W211 Q212 H213 W214 I217 M218 E219 S220

P223 C231 V232 V233 E234 N235 E236 Y237 Y244 H245 L246 D247 V248 V249 E250 R251 R255 P256 I257 L258 P263 S267 V270 G271 V274 E275 F276 V277 C278 S282 P286 Q289 W290 H293 VAL GLU LYS ASN GLY SER LYS TYR GLY PRO ASP GLY LEU PRO

TYR LEU K310 V311 L312 A315 T319 T320 D321 K322 E323 I324 E325 V326 L327 Y328 I329 R330 N331 V332 A337 Y340 G345 N346 S347 I350 A355 W356 L357 T358 V359 L360 PRO ALA PRO GLY ARG GLU

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

Chain E: 60% 40%

SGN1 IDS2 SGN3 IDS4 SGN5 IDS6 SGN7 IDS8 SGN9 IDS10

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	195.90Å 195.90Å 68.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.20 – 2.80	Depositor
% Data completeness (in resolution range)	98.3 (24.20-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.274 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5247	wwPDB-VP
Average B, all atoms (Å^2)	69.0	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: SO4, IDS, NI, SGN

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	0.42	0/1002	0.71	0/1360
1	C	0.44	0/1040	0.70	0/1407
2	B	0.44	0/1544	0.70	0/2109
2	D	0.46	0/1539	0.70	0/2102
All	All	0.44	0/5125	0.70	0/6978

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	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	979	0	932	86	0
1	C	1017	0	982	56	0
2	B	1505	0	1419	81	0
2	D	1500	0	1412	83	0
3	E	175	0	56	8	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	10	0	0	0	0
5	D	15	0	0	2	0
6	A	7	0	0	3	0
6	B	12	0	0	5	0
6	C	7	0	0	0	0
6	D	15	0	0	3	0
All	All	5247	0	4801	296	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 30.

All (296) 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:B:345:GLY:HA3	2:B:350:ILE:HG22	1.34	1.05
2:D:274:VAL:HG21	2:D:357:LEU:HD13	1.46	0.97
2:B:277:VAL:HG22	2:B:326:VAL:HG12	1.50	0.92
2:D:345:GLY:HA3	2:D:350:ILE:HG22	1.56	0.86
1:A:24:ARG:HG3	1:A:41:HIS:O	1.74	0.86
1:C:119:ARG:HH21	3:E:4:IDS:H2	1.41	0.84
2:B:211:ASN:N	2:B:211:ASN:HD22	1.78	0.82
2:D:176:LYS:HE3	2:D:217:ILE:HD11	1.64	0.79
2:B:274:VAL:HG21	2:B:357:LEU:HD13	1.65	0.77
1:A:74:TYR:HE1	1:A:76:SER:HB2	1.51	0.76
2:B:211:ASN:N	2:B:211:ASN:ND2	2.32	0.76
2:B:245:HIS:HB2	6:B:510:HOH:O	1.86	0.75
2:D:263:PRO:HB2	2:D:355:ALA:HB2	1.70	0.74
2:D:223:PRO:HA	2:D:248:VAL:HG11	1.69	0.72
2:D:282:SER:HB3	2:D:286:PRO:HG3	1.71	0.72
1:C:11:PRO:O	1:C:137:VAL:HG22	1.89	0.71
2:D:223:PRO:HA	2:D:248:VAL:CG1	2.21	0.70
2:D:337:ALA:HB2	2:D:359:VAL:HG23	1.73	0.70
2:B:211:ASN:ND2	2:B:211:ASN:H	1.86	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:GLN:HG2	2:D:213:HIS:CD2	2.24	0.70
2:D:274:VAL:CG1	2:D:329:ILE:HB	2.22	0.70
1:C:107:TRP:CZ2	1:C:121:PRO:HG3	2.28	0.69
2:B:321:ASP:O	2:B:324:ILE:HG22	1.92	0.69
2:B:256:PRO:HG2	2:B:345:GLY:HA2	1.74	0.69
1:A:87:GLU:HG3	1:A:97:TYR:CE1	2.29	0.68
1:A:35:ARG:NH1	2:B:164:LYS:HA	2.07	0.67
2:B:230:THR:HG23	2:B:242:HIS:O	1.95	0.67
1:C:123:THR:HA	1:C:127:GLN:OE1	1.95	0.67
2:D:321:ASP:O	2:D:324:ILE:HG22	1.96	0.66
1:C:92:ASN:OD1	1:C:94:TYR:HD2	1.79	0.66
1:C:118:LYS:HE3	1:C:122:ARG:O	1.96	0.65
1:A:64:TYR:CE1	1:A:79:PRO:HG3	2.32	0.65
1:A:73:LEU:HD11	1:A:109:VAL:HG13	1.77	0.65
1:C:35:ARG:NH1	2:D:163:GLU:O	2.30	0.64
2:B:350:ILE:HD12	2:B:350:ILE:O	1.97	0.64
1:C:27:PRO:HG3	1:C:41:HIS:NE2	2.13	0.64
1:C:12:LYS:NZ	1:C:46:LEU:HD12	2.12	0.64
1:C:105:LYS:HD3	1:C:107:TRP:CZ2	2.33	0.63
1:A:113:LYS:HE2	3:E:7:SGN:H3	1.80	0.63
1:C:12:LYS:CE	1:C:46:LEU:HD12	2.29	0.63
2:B:223:PRO:HA	2:B:248:VAL:HG13	1.79	0.63
2:B:236:GLU:HG3	2:B:237:TYR:CD1	2.34	0.62
2:B:345:GLY:HA3	2:B:350:ILE:CG2	2.22	0.61
1:C:18:ASN:HB2	1:C:128:LYS:O	2.00	0.61
1:A:67:MET:SD	1:A:71:GLY:HA2	2.41	0.61
1:C:92:ASN:O	1:C:93:HIS:HB2	2.00	0.61
2:D:171:ALA:O	2:D:172:ALA:HB3	2.01	0.61
2:D:329:ILE:HD11	2:D:340:TYR:CE2	2.35	0.61
2:B:176:LYS:HE3	2:B:178:ARG:HD3	1.83	0.60
1:A:72:LEU:HD21	1:A:119:ARG:HG2	1.82	0.60
2:D:257:ILE:HA	6:D:502:HOH:O	2.02	0.60
1:C:61:THR:O	1:C:63:GLN:HG3	2.02	0.59
1:A:59:THR:HG22	1:A:59:THR:O	2.02	0.59
2:D:167:HIS:O	2:D:246:LEU:HD12	2.02	0.59
2:B:236:GLU:HG3	2:B:237:TYR:CE1	2.38	0.59
2:D:320:THR:OG1	2:D:323:GLU:HG3	2.01	0.59
2:D:152:ARG:HG3	2:D:152:ARG:HH11	1.68	0.59
1:A:64:TYR:CZ	1:A:79:PRO:HG3	2.38	0.58
1:A:130:ILE:HG13	1:A:131:LEU:HD23	1.86	0.58
2:D:236:GLU:HG3	2:D:237:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PRO:HD2	2:B:251:ARG:NH1	2.19	0.58
2:B:256:PRO:HG2	2:B:345:GLY:CA	2.34	0.58
2:D:235:ASN:OD1	2:D:235:ASN:C	2.42	0.58
2:B:210:ARG:NH2	2:B:212:GLN:CB	2.66	0.58
2:B:337:ALA:HB2	2:B:359:VAL:HG23	1.86	0.58
1:C:31:VAL:HG23	1:C:74:TYR:HA	1.85	0.57
1:A:34:THR:OG1	1:A:35:ARG:N	2.38	0.57
2:B:171:ALA:O	2:B:172:ALA:HB3	2.03	0.57
2:D:271:GLY:O	2:D:331:ASN:ND2	2.38	0.57
2:D:186:MET:HE2	2:D:214:TRP:HZ2	1.69	0.57
2:B:180:PRO:HA	2:B:214:TRP:CD1	2.40	0.57
2:B:258:LEU:CD1	2:B:280:VAL:HG22	2.35	0.56
1:A:119:ARG:HD2	3:E:3:SGN:O1S	2.06	0.56
1:A:110:GLY:O	1:A:111:LEU:HG	2.06	0.56
1:C:14:LEU:HG	1:C:44:LEU:HD12	1.86	0.56
1:C:64:TYR:CZ	1:C:79:PRO:HG3	2.40	0.56
2:B:222:VAL:O	2:B:248:VAL:HG11	2.05	0.56
2:B:350:ILE:HD12	2:B:350:ILE:C	2.26	0.55
1:A:27:PRO:HG3	1:A:41:HIS:NE2	2.21	0.55
1:A:35:ARG:HH11	2:B:164:LYS:HA	1.70	0.55
1:C:68:ASP:OD2	1:C:72:LEU:HB3	2.07	0.55
1:C:89:LEU:HD13	1:C:95:ASN:OD1	2.08	0.54
1:C:61:THR:HB	1:C:63:GLN:HG3	1.89	0.54
1:A:124:HIS:ND1	1:A:125:TYR:N	2.56	0.54
2:B:160:GLU:HG2	2:B:161:LYS:N	2.22	0.54
2:B:207:TYR:CD2	2:B:216:LEU:HD11	2.43	0.54
2:B:329:ILE:HD11	2:B:340:TYR:CE2	2.43	0.54
1:C:12:LYS:HE3	1:C:46:LEU:HD12	1.90	0.54
2:D:350:ILE:HD12	2:D:350:ILE:C	2.28	0.54
1:A:57:LYS:HA	1:A:63:GLN:O	2.08	0.54
1:C:89:LEU:HD13	2:D:251:ARG:NH2	2.23	0.54
1:A:24:ARG:NH1	1:A:39:ASP:OD2	2.40	0.53
1:A:98:ILE:CG2	1:A:99:SER:N	2.70	0.53
2:B:274:VAL:HG21	2:B:357:LEU:CD1	2.36	0.53
2:B:353:HIS:HE1	6:B:511:HOH:O	1.90	0.53
1:A:112:LYS:O	1:A:114:ASN:N	2.42	0.53
2:D:267:SER:HA	2:D:358:THR:O	2.08	0.53
2:B:184:ASN:HA	2:B:185:PRO:C	2.28	0.53
1:A:58:SER:O	1:A:62:GLY:HA2	2.09	0.53
1:C:25:ILE:O	1:C:41:HIS:HB3	2.09	0.53
2:D:274:VAL:HG12	2:D:329:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HG3	3:E:6:IDS:O2S	2.09	0.53
2:B:157:THR:CG2	2:B:181:ALA:C	2.77	0.53
2:D:256:PRO:HG2	2:D:345:GLY:HA2	1.89	0.53
1:A:42:ILE:O	1:A:44:LEU:HG	2.09	0.53
1:C:50:SER:HB3	1:C:53:GLU:CD	2.30	0.53
1:A:72:LEU:CD2	1:A:119:ARG:HG2	2.38	0.53
1:C:57:LYS:HA	1:C:63:GLN:O	2.09	0.53
1:A:105:LYS:O	1:A:106:ASN:HB2	2.08	0.52
1:A:95:ASN:HB3	1:A:97:TYR:HE1	1.74	0.52
2:B:188:THR:HG22	2:B:234:GLU:O	2.10	0.52
1:C:58:SER:C	1:C:60:GLU:H	2.14	0.52
1:A:71:GLY:HA3	1:A:121:PRO:HD3	1.91	0.52
2:B:157:THR:HG23	2:B:181:ALA:C	2.30	0.52
2:D:236:GLU:HG3	2:D:237:TYR:CD1	2.45	0.51
2:D:315:ALA:HA	2:D:319:THR:OG1	2.11	0.51
1:A:127:GLN:O	1:A:130:ILE:HG12	2.11	0.51
1:A:31:VAL:HG23	1:A:74:TYR:HA	1.92	0.51
2:B:176:LYS:HG3	2:B:217:ILE:HG12	1.92	0.51
2:D:176:LYS:HE3	2:D:217:ILE:CD1	2.37	0.51
1:A:12:LYS:CE	1:A:46:LEU:HD12	2.39	0.51
2:D:181:ALA:HB1	2:D:233:VAL:HG11	1.93	0.51
1:A:46:LEU:HD23	1:A:56:ILE:HG12	1.92	0.51
1:A:69:THR:O	1:A:69:THR:HG22	2.08	0.51
2:B:210:ARG:NH1	2:B:211:ASN:ND2	2.59	0.51
2:D:172:ALA:O	2:D:220:SER:HA	2.09	0.51
2:D:177:PHE:HB3	2:D:244:TYR:CD2	2.46	0.51
2:D:274:VAL:HG13	2:D:329:ILE:HB	1.91	0.51
1:A:112:LYS:HA	3:E:6:IDS:O3S	2.11	0.51
1:A:46:LEU:CD2	1:A:56:ILE:HG12	2.41	0.50
2:B:216:LEU:HD12	2:B:217:ILE:H	1.75	0.50
1:C:34:THR:OG1	1:C:35:ARG:N	2.44	0.50
1:A:53:GLU:OE2	1:A:100:LYS:HE3	2.11	0.50
1:C:94:TYR:OH	2:D:169:VAL:HG12	2.12	0.50
1:A:71:GLY:O	1:A:119:ARG:HA	2.11	0.50
2:D:174:THR:OG1	2:D:219:GLU:HA	2.11	0.50
2:B:171:ALA:O	2:B:172:ALA:CB	2.60	0.50
2:B:188:THR:O	2:B:233:VAL:HA	2.12	0.49
1:C:80:ASN:O	1:C:83:CYS:HB2	2.11	0.49
1:A:91:GLU:HG3	6:A:305:HOH:O	2.11	0.49
1:A:117:CYS:SG	1:A:118:LYS:N	2.85	0.49
2:D:276:PHE:HZ	2:D:357:LEU:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ALA:HA	1:C:82:GLU:O	2.12	0.49
1:A:42:ILE:O	1:A:44:LEU:N	2.42	0.49
2:B:223:PRO:HA	2:B:248:VAL:CG1	2.42	0.49
1:C:105:LYS:O	1:C:106:ASN:HB2	2.12	0.49
2:D:154:PRO:HA	2:D:182:GLY:O	2.13	0.49
2:D:191:TRP:O	2:D:192:LEU:HD12	2.11	0.49
2:D:276:PHE:CZ	2:D:357:LEU:HB2	2.48	0.49
2:D:337:ALA:HB2	2:D:359:VAL:CG2	2.42	0.49
1:A:123:THR:HG22	1:A:124:HIS:N	2.26	0.49
2:B:345:GLY:CA	2:B:350:ILE:HG22	2.25	0.49
1:A:112:LYS:NZ	1:A:122:ARG:HH21	2.10	0.48
2:B:190:ARG:HD3	2:B:234:GLU:OE2	2.13	0.48
2:D:213:HIS:CE1	6:D:501:HOH:O	2.64	0.48
2:D:321:ASP:HA	2:D:324:ILE:HG22	1.94	0.48
2:B:254:HIS:HA	2:B:348:ILE:HG21	1.95	0.48
2:B:274:VAL:HG22	2:B:275:GLU:N	2.28	0.48
2:D:152:ARG:HG3	2:D:152:ARG:NH1	2.29	0.48
2:B:176:LYS:HD3	2:B:217:ILE:HD11	1.94	0.48
2:B:200:GLN:HA	2:B:207:TYR:CE1	2.49	0.48
1:A:74:TYR:CE1	1:A:76:SER:HB2	2.39	0.48
1:A:105:LYS:O	1:A:106:ASN:CB	2.61	0.48
1:A:124:HIS:CG	1:A:125:TYR:N	2.82	0.48
1:A:134:PRO:HD2	2:B:251:ARG:HH12	1.77	0.48
2:B:219:GLU:O	2:B:220:SER:C	2.52	0.48
2:D:277:VAL:HG22	2:D:326:VAL:HG12	1.95	0.48
2:B:333:THR:O	2:B:359:VAL:HG21	2.14	0.47
1:A:98:ILE:HD13	1:A:106:ASN:HA	1.95	0.47
2:D:213:HIS:HE1	6:D:501:HOH:O	1.97	0.47
1:C:64:TYR:CE1	1:C:79:PRO:HG3	2.49	0.47
1:A:12:LYS:HE3	1:A:46:LEU:HD12	1.97	0.47
1:A:92:ASN:OD1	1:A:94:TYR:HD2	1.97	0.47
1:A:113:LYS:NZ	6:A:303:HOH:O	2.45	0.47
2:D:155:TYR:CE1	2:D:182:GLY:C	2.88	0.47
2:D:174:THR:HG23	2:D:218:MET:O	2.15	0.47
2:D:177:PHE:HB3	2:D:244:TYR:CE2	2.50	0.47
2:D:329:ILE:HG22	2:D:329:ILE:O	2.14	0.47
1:A:26:LEU:HD12	1:A:30:THR:HB	1.96	0.47
1:C:61:THR:O	1:C:62:GLY:C	2.53	0.47
1:C:50:SER:HB3	1:C:53:GLU:OE1	2.15	0.47
2:B:353:HIS:CE1	6:B:511:HOH:O	2.66	0.46
1:A:113:LYS:CE	3:E:7:SGN:H3	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:326:VAL:HG23	2:D:326:VAL:O	2.16	0.46
1:A:73:LEU:CD1	1:A:109:VAL:HG13	2.43	0.46
2:B:176:LYS:HG3	2:B:217:ILE:CG1	2.45	0.46
1:C:64:TYR:CE2	1:C:79:PRO:HG3	2.51	0.46
2:D:255:ARG:NE	5:D:401:SO4:O4	2.48	0.46
1:A:43:GLN:HE21	1:A:43:GLN:HB3	1.55	0.46
2:D:278:CYS:O	2:D:325:GLU:HG3	2.16	0.46
2:B:207:TYR:CD2	2:B:216:LEU:CD1	2.99	0.46
1:C:80:ASN:O	1:C:83:CYS:N	2.49	0.46
1:A:65:LEU:O	1:A:85:PHE:HE2	1.98	0.45
1:A:113:LYS:HE3	3:E:6:IDS:O2S	2.16	0.45
1:A:98:ILE:HG23	1:A:99:SER:N	2.31	0.45
1:C:18:ASN:HB2	1:C:129:ALA:HA	1.98	0.45
1:A:58:SER:C	1:A:60:GLU:H	2.19	0.45
1:A:97:TYR:CD1	1:A:97:TYR:N	2.84	0.45
2:B:262:LEU:HA	2:B:263:PRO:C	2.37	0.45
2:B:340:TYR:N	2:B:340:TYR:CD1	2.84	0.45
1:C:89:LEU:HD13	2:D:251:ARG:HH22	1.80	0.45
2:D:198:PHE:CE2	2:D:207:TYR:CD2	3.04	0.45
2:D:251:ARG:HD2	2:D:251:ARG:HA	1.80	0.45
1:A:112:LYS:HD2	1:A:118:LYS:HD2	1.98	0.45
1:C:105:LYS:HD3	1:C:107:TRP:CE2	2.51	0.45
2:D:267:SER:OG	2:D:358:THR:HB	2.16	0.45
1:A:54:VAL:HG21	1:A:87:GLU:HB2	1.97	0.45
2:D:290:TRP:NE1	2:D:327:LEU:HB2	2.32	0.45
1:A:119:ARG:HB3	1:A:121:PRO:HD2	1.99	0.45
2:B:256:PRO:CG	2:B:345:GLY:HA2	2.46	0.44
1:C:64:TYR:HB2	1:C:83:CYS:SG	2.57	0.44
1:C:102:HIS:HB3	1:C:105:LYS:HD2	1.98	0.44
2:B:178:ARG:HD2	2:B:215:SER:HB3	1.98	0.44
2:B:269:VAL:HA	2:B:360:LEU:O	2.17	0.44
2:D:186:MET:HE2	2:D:187:PRO:HD2	1.99	0.44
2:D:204:ILE:HD12	2:D:205:GLY:N	2.32	0.44
2:B:203:ARG:HD2	6:B:505:HOH:O	2.17	0.44
1:A:108:PHE:HB2	1:A:130:ILE:HG22	1.99	0.44
1:C:46:LEU:HD23	1:C:56:ILE:HG12	1.99	0.44
1:A:130:ILE:HG13	1:A:131:LEU:CD2	2.47	0.44
1:A:49:GLU:HA	1:A:49:GLU:OE1	2.18	0.44
1:A:124:HIS:CG	1:A:125:TYR:H	2.36	0.44
2:B:167:HIS:O	2:B:246:LEU:HD12	2.18	0.44
1:A:122:ARG:O	6:A:301:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:GLN:O	1:C:130:ILE:HG12	2.17	0.43
2:D:158:ASN:HB3	2:D:180:PRO:HG2	2.00	0.43
2:D:186:MET:CE	2:D:214:TRP:HZ2	2.31	0.43
1:C:98:ILE:CG2	1:C:99:SER:N	2.81	0.43
2:D:270:VAL:HA	2:D:332:VAL:HG23	2.00	0.43
2:D:326:VAL:HB	2:D:328:TYR:HE1	1.84	0.43
2:B:275:GLU:HG3	2:B:328:TYR:CD1	2.54	0.43
2:B:210:ARG:HH11	2:B:211:ASN:HD21	1.66	0.43
2:B:224:SER:HB2	6:B:502:HOH:O	2.19	0.43
1:C:43:GLN:OE1	1:C:137:VAL:HG13	2.19	0.43
1:A:125:TYR:O	1:A:130:ILE:HD11	2.18	0.43
1:C:61:THR:O	1:C:63:GLN:N	2.51	0.43
2:D:274:VAL:HG22	2:D:275:GLU:N	2.34	0.43
2:B:151:LYS:O	2:B:152:ARG:HB2	2.19	0.43
2:B:181:ALA:CB	2:B:233:VAL:HG11	2.49	0.43
1:C:41:HIS:HD1	1:C:41:HIS:H	1.67	0.43
1:C:49:GLU:HB3	1:C:50:SER:H	1.63	0.43
2:D:256:PRO:HG3	2:D:346:ASN:ND2	2.33	0.43
1:C:64:TYR:CB	1:C:83:CYS:SG	3.08	0.42
2:D:258:LEU:N	2:D:258:LEU:HD12	2.35	0.42
1:A:95:ASN:HB3	1:A:97:TYR:CE1	2.53	0.42
1:C:38:SER:O	1:C:39:ASP:C	2.58	0.42
1:A:73:LEU:HD21	1:A:109:VAL:HG22	2.01	0.42
2:B:286:PRO:HG2	2:B:288:ILE:HD11	2.01	0.42
2:D:186:MET:HE2	2:D:214:TRP:CZ2	2.53	0.42
2:D:199:LYS:H	2:D:202:HIS:CE1	2.38	0.42
1:A:14:LEU:HG	1:A:44:LEU:HD12	2.00	0.42
1:A:65:LEU:O	1:A:85:PHE:CE2	2.72	0.42
2:B:176:LYS:CD	2:B:217:ILE:HD11	2.49	0.42
2:D:191:TRP:CH2	2:D:231:CYS:HB3	2.54	0.42
1:A:14:LEU:O	1:A:132:PHE:HD2	2.02	0.42
1:A:123:THR:CG2	1:A:124:HIS:N	2.83	0.42
1:A:123:THR:HA	1:A:127:GLN:OE1	2.20	0.42
2:B:156:TRP:HA	2:B:156:TRP:CE3	2.55	0.42
2:B:157:THR:O	2:B:158:ASN:OD1	2.37	0.42
2:D:152:ARG:HB3	2:D:184:ASN:H	1.85	0.42
2:D:255:ARG:HG2	5:D:401:SO4:O1	2.20	0.42
1:C:15:TYR:CE1	2:D:168:ALA:HB3	2.55	0.42
2:D:193:LYS:O	2:D:194:ASN:C	2.58	0.42
1:A:89:LEU:O	2:B:257:ILE:HD13	2.20	0.41
2:B:287:HIS:O	2:B:344:ALA:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:326:VAL:HB	2:D:328:TYR:CE1	2.55	0.41
1:A:15:TYR:CZ	2:B:168:ALA:HB3	2.55	0.41
2:B:164:LYS:HE2	2:B:167:HIS:NE2	2.35	0.41
2:B:179:CYS:O	2:B:214:TRP:HB3	2.20	0.41
2:D:197:GLU:O	2:D:202:HIS:CE1	2.73	0.41
1:A:66:ALA:HB3	1:A:74:TYR:CE1	2.56	0.41
1:C:67:MET:CG	1:C:71:GLY:HA2	2.50	0.41
2:B:221:VAL:HG12	2:B:248:VAL:HG21	2.02	0.41
2:D:155:TYR:CZ	2:D:182:GLY:HA3	2.55	0.41
3:E:3:SGN:O3	3:E:4:IDS:O5	2.35	0.41
2:B:179:CYS:N	2:B:180:PRO:HD3	2.36	0.41
2:B:342:CYS:O	2:B:352:PHE:HA	2.21	0.41
1:A:64:TYR:CD1	1:A:79:PRO:HG3	2.55	0.41
1:C:23:LEU:HB3	1:C:44:LEU:HD11	2.03	0.41
1:C:134:PRO:O	1:C:135:LEU:HD23	2.20	0.41
1:A:69:THR:HA	1:A:102:HIS:CE1	2.56	0.41
1:A:108:PHE:HB2	1:A:130:ILE:CG2	2.51	0.41
1:C:23:LEU:HD21	1:C:65:LEU:HD22	2.02	0.41
2:D:184:ASN:HA	2:D:185:PRO:C	2.42	0.41
2:D:223:PRO:HA	2:D:248:VAL:HG13	1.99	0.41
2:B:337:ALA:HB2	2:B:359:VAL:CG2	2.48	0.41
2:D:329:ILE:HD11	2:D:340:TYR:HE2	1.81	0.41
1:A:90:GLU:OE2	1:A:125:TYR:CE1	2.74	0.40
2:B:329:ILE:HG22	2:B:332:VAL:HG12	2.03	0.40
1:A:21:HIS:HB3	1:A:34:THR:O	2.20	0.40
2:B:237:TYR:CD1	2:B:237:TYR:N	2.87	0.40
1:A:23:LEU:HA	1:A:23:LEU:HD12	1.90	0.40
2:D:193:LYS:HB2	2:D:198:PHE:CD1	2.56	0.40
2:D:223:PRO:CA	2:D:248:VAL:HG11	2.47	0.40
1:C:61:THR:HG21	1:C:63:GLN:OE1	2.21	0.40
2:D:171:ALA:O	2:D:172:ALA:CB	2.67	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	127/140 (91%)	101 (80%)	19 (15%)	7 (6%)	2 5
1	C	128/140 (91%)	105 (82%)	16 (12%)	7 (6%)	2 5
2	B	193/219 (88%)	168 (87%)	21 (11%)	4 (2%)	7 23
2	D	192/219 (88%)	166 (86%)	21 (11%)	5 (3%)	5 18
All	All	640/718 (89%)	540 (84%)	77 (12%)	23 (4%)	3 11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	113	LYS
2	B	317	VAL
2	B	332	VAL
2	D	312	LEU
1	A	43	GLN
1	A	81	GLU
1	A	136	PRO
2	B	158	ASN
1	C	18	ASN
1	C	41	HIS
1	C	49	GLU
1	C	113	LYS
2	D	206	GLY
2	D	347	SER
2	D	331	ASN
1	C	68	ASP
1	C	117	CYS
1	A	119	ARG
1	C	62	GLY
2	B	329	ILE
2	D	154	PRO
1	A	62	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/123 (81%)	96 (96%)	4 (4%)	31	65
1	C	109/123 (89%)	106 (97%)	3 (3%)	43	77
2	B	155/186 (83%)	148 (96%)	7 (4%)	27	60
2	D	155/186 (83%)	144 (93%)	11 (7%)	14	39
All	All	519/618 (84%)	494 (95%)	25 (5%)	25	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	90	GLU
1	A	117	CYS
1	A	136	PRO
2	B	164	LYS
2	B	190	ARG
2	B	192	LEU
2	B	211	ASN
2	B	253	PRO
2	B	347	SER
2	B	356	TRP
1	C	9	LYS
1	C	61	THR
1	C	117	CYS
2	D	158	ASN
2	D	159	THR
2	D	163	GLU
2	D	210	ARG
2	D	212	GLN
2	D	250	GLU
2	D	255	ARG
2	D	289	GLN
2	D	312	LEU
2	D	347	SER
2	D	356	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
2	B	200	GLN
2	B	211	ASN
2	B	259	GLN
2	B	331	ASN
2	D	158	ASN
2	D	202	HIS
2	D	213	HIS
2	D	289	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	SGN	E	1	3	19,20,20	2.20	6 (31%)	24,31,31	1.14	1 (4%)
3	IDS	E	10	3	15,15,17	2.44	5 (33%)	15,22,26	3.01	6 (40%)
3	IDS	E	2	3	16,16,17	1.64	5 (31%)	17,24,26	2.44	5 (29%)
3	SGN	E	3	3	18,19,20	1.96	5 (27%)	22,29,31	1.13	1 (4%)
3	IDS	E	4	3	16,16,17	1.66	5 (31%)	17,24,26	2.56	5 (29%)
3	SGN	E	5	3	18,19,20	2.36	5 (27%)	22,29,31	1.04	1 (4%)
3	IDS	E	6	3	16,16,17	1.45	3 (18%)	17,24,26	2.32	6 (35%)
3	SGN	E	7	3	18,19,20	1.91	5 (27%)	22,29,31	1.03	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IDS	E	8	3	16,16,17	1.39	3 (18%)	17,24,26	2.42	3 (17%)
3	SGN	E	9	3	18,19,20	2.04	6 (33%)	22,29,31	1.12	2 (9%)

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	-	0/11/31/31	0/1/1/1
3	IDS	E	10	3	-	4/9/22/29	0/1/1/1
3	IDS	E	2	3	-	0/9/26/29	0/1/1/1
3	SGN	E	3	3	-	6/11/28/31	0/1/1/1
3	IDS	E	4	3	-	1/9/26/29	0/1/1/1
3	SGN	E	5	3	-	5/11/28/31	0/1/1/1
3	IDS	E	6	3	-	2/9/26/29	0/1/1/1
3	SGN	E	7	3	-	7/11/28/31	0/1/1/1
3	IDS	E	8	3	-	5/9/26/29	0/1/1/1
3	SGN	E	9	3	-	3/11/28/31	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	SGN	S1-N2	6.22	1.67	1.59
3	E	10	IDS	C4-C5	5.66	1.61	1.52
3	E	5	SGN	S1-N2	5.61	1.67	1.59
3	E	3	SGN	S1-N2	5.26	1.66	1.59
3	E	10	IDS	O5-C5	4.96	1.52	1.43
3	E	5	SGN	O2S-S1	4.87	1.47	1.42
3	E	9	SGN	C1-C2	4.84	1.59	1.52
3	E	7	SGN	S1-N2	4.72	1.65	1.59
3	E	5	SGN	C1-C2	3.98	1.58	1.52
3	E	9	SGN	S1-N2	3.90	1.64	1.59
3	E	1	SGN	C1-C2	3.80	1.57	1.52
3	E	10	IDS	C5-C6	3.65	1.55	1.52
3	E	7	SGN	O2S-S1	3.56	1.46	1.42
3	E	8	IDS	C4-C5	3.26	1.58	1.53
3	E	5	SGN	O1S-S1	3.23	1.45	1.42
3	E	7	SGN	C1-C2	3.17	1.57	1.52
3	E	1	SGN	O2S-S1	3.17	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	IDS	O2-C2	-3.14	1.42	1.47
3	E	3	SGN	O1S-S1	3.08	1.45	1.42
3	E	9	SGN	C4-C5	2.88	1.59	1.53
3	E	9	SGN	O2S-S1	2.88	1.45	1.42
3	E	9	SGN	O1S-S1	2.74	1.45	1.42
3	E	10	IDS	O2-C2	-2.74	1.43	1.47
3	E	2	IDS	C4-C5	2.73	1.57	1.53
3	E	1	SGN	O1S-S1	2.70	1.45	1.42
3	E	4	IDS	C1-C2	2.70	1.56	1.51
3	E	2	IDS	C1-C2	2.63	1.55	1.51
3	E	3	SGN	O2S-S1	2.62	1.45	1.42
3	E	7	SGN	O1S-S1	2.62	1.45	1.42
3	E	4	IDS	O2-C2	-2.62	1.43	1.47
3	E	8	IDS	O6B-C6	-2.60	1.22	1.30
3	E	6	IDS	O6B-C6	-2.58	1.22	1.30
3	E	4	IDS	O6B-C6	-2.53	1.22	1.30
3	E	2	IDS	O6B-C6	-2.48	1.22	1.30
3	E	6	IDS	C1-C2	2.43	1.55	1.51
3	E	6	IDS	C4-C5	2.38	1.57	1.53
3	E	10	IDS	O6B-C6	-2.35	1.22	1.30
3	E	4	IDS	O5-C5	2.34	1.47	1.43
3	E	5	SGN	O5-C5	2.29	1.48	1.43
3	E	3	SGN	O4-C4	2.27	1.48	1.43
3	E	2	IDS	C3-C2	2.27	1.57	1.53
3	E	1	SGN	C4-C5	2.26	1.57	1.53
3	E	4	IDS	O4-C4	-2.23	1.37	1.43
3	E	9	SGN	O5-C5	2.19	1.47	1.43
3	E	7	SGN	C4-C5	2.08	1.57	1.53
3	E	3	SGN	C4-C3	2.07	1.57	1.52
3	E	1	SGN	C3-C2	2.00	1.57	1.53
3	E	8	IDS	O2-S	2.00	1.63	1.57

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	10	IDS	C2-O2-S	9.48	130.28	117.91
3	E	4	IDS	C2-O2-S	8.47	128.96	117.91
3	E	8	IDS	C2-O2-S	8.34	128.79	117.91
3	E	2	IDS	C2-O2-S	7.79	128.07	117.91
3	E	6	IDS	C2-O2-S	7.40	127.56	117.91
3	E	2	IDS	C1-C2-C3	3.89	115.21	109.40
3	E	1	SGN	O1S-S1-O2S	-3.21	112.56	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	10	IDS	O6B-C6-C5	3.04	121.72	113.03
3	E	3	SGN	O1S-S1-O2S	-3.02	113.03	120.16
3	E	9	SGN	O1S-S1-O2S	-2.99	113.10	120.16
3	E	4	IDS	O4-C4-C5	-2.95	103.13	109.74
3	E	4	IDS	O6B-C6-O6A	-2.85	117.61	124.09
3	E	10	IDS	O6B-C6-O6A	-2.85	117.62	124.09
3	E	10	IDS	C3-C4-C5	2.82	114.86	109.81
3	E	8	IDS	O6B-C6-O6A	-2.79	117.74	124.09
3	E	2	IDS	O6B-C6-O6A	-2.78	117.77	124.09
3	E	5	SGN	O1S-S1-O2S	-2.77	113.61	120.16
3	E	6	IDS	O6B-C6-O6A	-2.72	117.92	124.09
3	E	7	SGN	O1S-S1-O2S	-2.66	113.87	120.16
3	E	6	IDS	O4-C4-C3	-2.65	104.22	110.35
3	E	4	IDS	C4-C3-C2	2.62	114.92	110.24
3	E	10	IDS	C1-C2-C3	-2.46	106.46	109.94
3	E	10	IDS	C1-O5-C5	2.40	117.59	113.92
3	E	6	IDS	O4-C4-C5	-2.27	104.65	109.74
3	E	4	IDS	O6B-C6-C5	2.20	121.70	113.65
3	E	6	IDS	O6B-C6-C5	2.17	121.58	113.65
3	E	9	SGN	C4-C3-C2	-2.14	107.89	111.02
3	E	8	IDS	O6B-C6-C5	2.10	121.32	113.65
3	E	6	IDS	C4-C3-C2	2.09	113.97	110.24
3	E	7	SGN	O2S-S1-N2	-2.05	105.12	108.87
3	E	2	IDS	O2-C2-C3	2.03	109.78	106.95
3	E	2	IDS	C4-C3-C2	2.00	113.81	110.24

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	SGN	C4-C5-C6-O6
3	E	3	SGN	O5-C5-C6-O6
3	E	3	SGN	C6-O6-S2-O4S
3	E	4	IDS	C3-C2-O2-S
3	E	5	SGN	C2-N2-S1-O2S
3	E	5	SGN	C2-N2-S1-O3S
3	E	6	IDS	C1-C2-O2-S
3	E	6	IDS	C3-C2-O2-S
3	E	7	SGN	O5-C5-C6-O6
3	E	8	IDS	C1-C2-O2-S
3	E	8	IDS	C3-C2-O2-S
3	E	8	IDS	C2-O2-S-O1S

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Mol	Chain	Res	Type	Atoms
3	E	8	IDS	C2-O2-S-O2S
3	E	8	IDS	C2-O2-S-O3S
3	E	9	SGN	C2-N2-S1-O1S
3	E	9	SGN	C2-N2-S1-O3S
3	E	10	IDS	O5-C5-C6-O6A
3	E	5	SGN	O5-C5-C6-O6
3	E	3	SGN	C6-O6-S2-O6S
3	E	10	IDS	C2-O2-S-O1S
3	E	7	SGN	C6-O6-S2-O4S
3	E	7	SGN	C6-O6-S2-O5S
3	E	3	SGN	C6-O6-S2-O5S
3	E	7	SGN	C4-C5-C6-O6
3	E	7	SGN	C6-O6-S2-O6S
3	E	5	SGN	C4-C5-C6-O6
3	E	3	SGN	C2-N2-S1-O2S
3	E	5	SGN	C2-N2-S1-O1S
3	E	7	SGN	C3-C2-N2-S1
3	E	10	IDS	C2-O2-S-O2S
3	E	10	IDS	C2-O2-S-O3S
3	E	7	SGN	C5-C6-O6-S2
3	E	9	SGN	C2-N2-S1-O2S

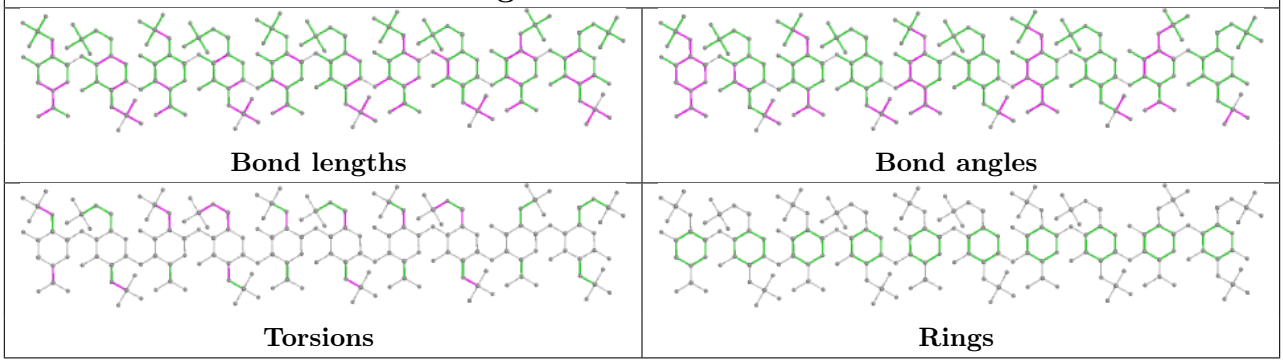
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	IDS	2	0
3	E	6	IDS	3	0
3	E	3	SGN	2	0
3	E	7	SGN	2	0

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

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	C	202	-	4,4,4	0.40	0	6,6,6	0.37	0
5	SO4	C	201	-	4,4,4	0.22	0	6,6,6	0.16	0
5	SO4	D	403	-	4,4,4	0.56	0	6,6,6	0.15	0
5	SO4	D	401	-	4,4,4	0.23	0	6,6,6	0.19	0
5	SO4	D	402	-	4,4,4	0.47	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	SO4	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.