



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:22 PM UTC

PDB ID : 2O39 / pdb_00002o39
Title : Human Adenovirus type 11 knob in complex with domains SCR1 and SCR2 of CD46 (membrane cofactor protein, MCP)
Authors : Persson, D.B.; Reiter, D.M.; Arnberg, N.; Stehle, T.
Deposited on : 2006-12-01
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

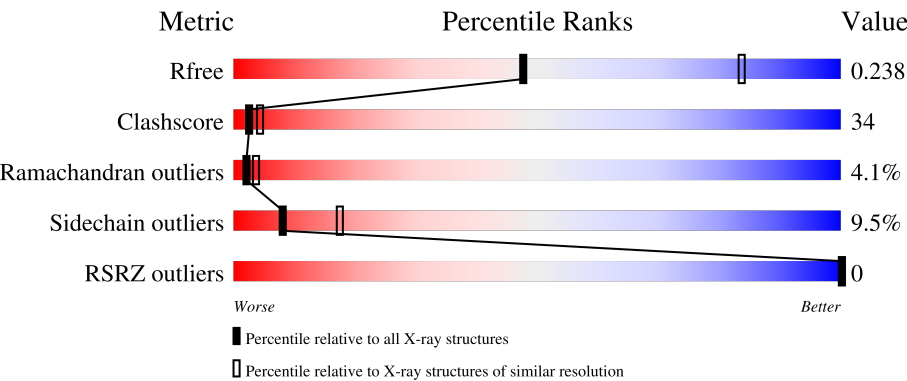
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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

Mol	Chain	Length	Quality of chain
1	A	197	52% 40% 6% .
1	B	197	54% 38% . .
2	C	126	44% 45% 7% .
2	D	126	39% 52% 8% .
3	E	3	33% 33% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	3	 33% 67%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5249 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.

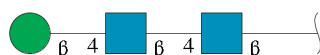
- Molecule 1 is a protein called Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1548	971	258	310	9			
1	B	197	Total	C	N	O	S	0	0	0
			1548	971	258	310	9			

- Molecule 2 is a protein called Membrane cofactor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	126	Total	C	N	O	S	0	0	0
			1019	659	160	190	10			
2	D	126	Total	C	N	O	S	0	0	0
			1019	659	160	190	10			

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



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Ca	0	0
			2	2		

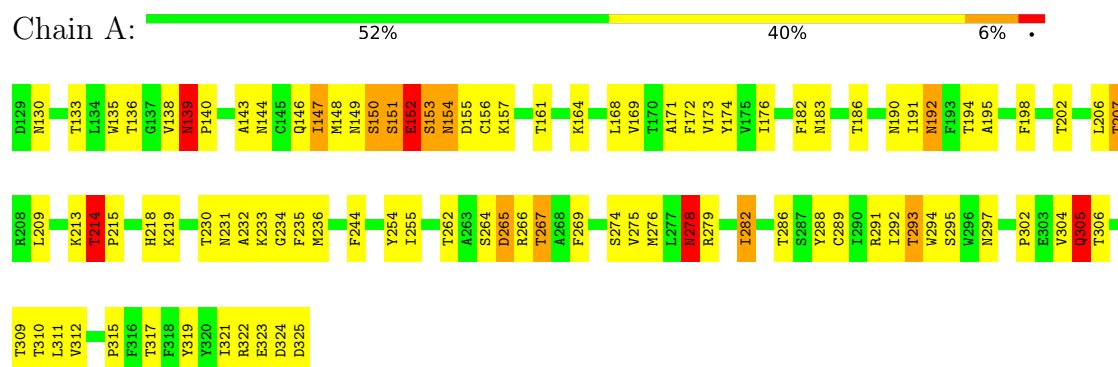
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	9	Total	O	0	0
			9	9		
5	C	7	Total	O	0	0
			7	7		
5	D	5	Total	O	0	0
			5	5		

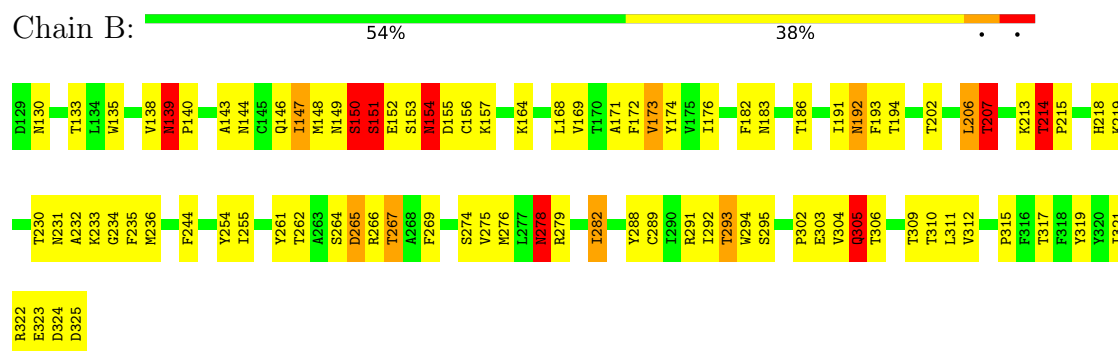
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

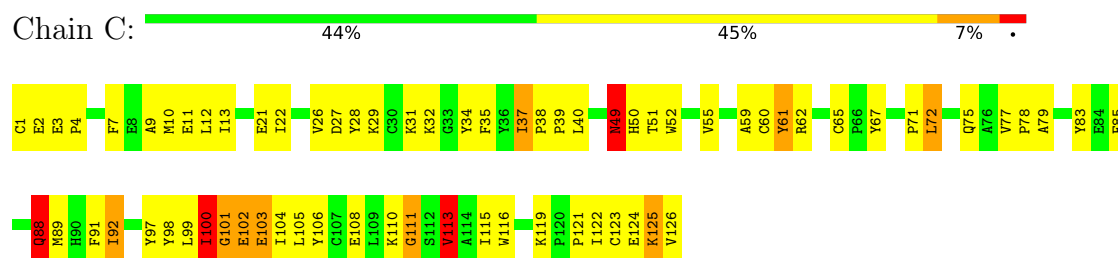
• Molecule 1: Fiber protein



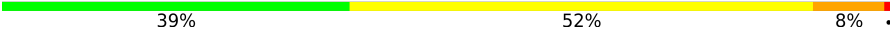
• Molecule 1: Fiber protein

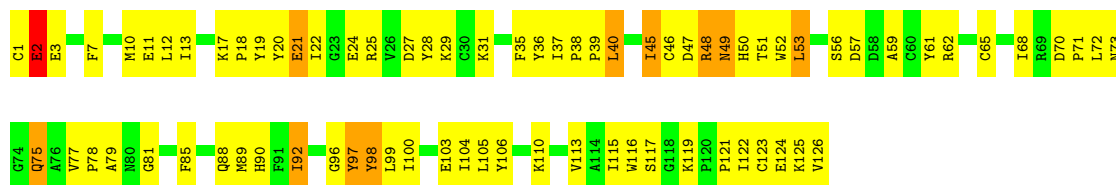


• Molecule 2: Membrane cofactor protein

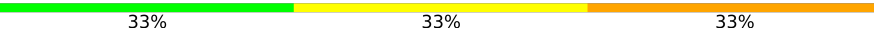


• Molecule 2: Membrane cofactor protein

Chain D:  39% 52% 8%



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

Chain E:  33% 33% 33%



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

Chain F:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	106.14Å 106.14Å 68.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.85 40.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.1 (40.00-2.85) 88.0 (40.00-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.273 0.237 , 0.238	Depositor DCC
R_{free} test set	2418 reflections (9.12%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.457 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5249	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA

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	0.49	0/1581	0.95	5/2156 (0.2%)
1	B	0.53	1/1581 (0.1%)	0.99	9/2156 (0.4%)
2	C	0.48	0/1053	0.89	3/1432 (0.2%)
2	D	0.42	0/1053	0.91	2/1432 (0.1%)
All	All	0.49	1/5268 (0.0%)	0.95	19/7176 (0.3%)

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	2
2	C	0	1
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	SER	CA-C	-6.00	1.45	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASN	CA-C-N	7.67	127.60	119.85
1	A	139	ASN	C-N-CA	7.67	127.60	119.85
1	B	139	ASN	CA-C-N	7.55	127.47	119.85
1	B	139	ASN	C-N-CA	7.55	127.47	119.85
2	D	119	LYS	CA-C-N	7.27	124.97	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	119	LYS	C-N-CA	7.27	124.97	119.66
1	A	214	THR	CA-C-N	6.58	128.07	119.84
1	A	214	THR	C-N-CA	6.58	128.07	119.84
1	B	214	THR	CA-C-N	6.44	127.89	119.84
1	B	214	THR	C-N-CA	6.44	127.89	119.84
1	B	207	THR	N-CA-C	6.13	117.97	111.28
1	B	254	TYR	N-CA-C	5.69	118.82	109.72
2	C	88	GLN	N-CA-C	5.46	117.49	109.24
1	A	254	TYR	N-CA-C	5.41	118.38	109.72
1	B	173	VAL	N-CA-C	5.21	115.87	108.42
2	C	111	GLY	N-CA-C	-5.19	106.90	111.67
1	B	150	SER	CA-C-N	-5.09	114.05	122.39
1	B	150	SER	C-N-CA	-5.09	114.05	122.39
2	C	113	VAL	N-CA-C	5.07	115.04	108.35

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLU	Peptide
1	A	153	SER	Peptide
2	C	49	ASN	Peptide
2	D	2	GLU	Peptide

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	1548	0	1487	82	1
1	B	1548	0	1487	83	1
2	C	1019	0	963	93	0
2	D	1019	0	965	92	0
3	E	39	0	34	1	0
3	F	39	0	34	3	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	13	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	9	0	0	3	0
5	C	7	0	0	1	0
5	D	5	0	0	2	0
All	All	5249	0	4970	348	2

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 34.

All (348) 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:1:CYS:SG	2:D:46:CYS:CB	2.25	1.24
2:C:99:LEU:HD11	2:C:103:GLU:HB3	1.35	1.07
2:C:1:CYS:N	2:C:50:HIS:HB3	1.72	1.03
2:D:62:ARG:HG3	2:D:85:PHE:CE2	2.01	0.96
2:C:101:GLY:O	2:C:102:GLU:O	1.85	0.94
1:A:130:ASN:HB3	1:A:219:LYS:HB3	1.49	0.93
2:C:99:LEU:CD1	2:C:103:GLU:HB3	1.97	0.93
2:D:1:CYS:CB	2:D:46:CYS:SG	2.57	0.92
1:B:130:ASN:HB3	1:B:219:LYS:HB3	1.49	0.92
2:C:12:LEU:HD11	2:C:26:VAL:HG22	1.53	0.91
2:C:1:CYS:H2	2:C:50:HIS:HB3	1.26	0.90
1:A:278:ASN:HB3	1:A:289:CYS:H	1.37	0.89
3:F:2:NAG:H3	3:F:2:NAG:H83	1.56	0.88
1:B:278:ASN:HB3	1:B:289:CYS:H	1.40	0.86
2:D:48:ARG:CD	2:D:48:ARG:H	1.89	0.85
2:C:100:ILE:HD11	2:C:122:ILE:H	1.46	0.81
1:A:146:GLN:NE2	1:A:152:GLU:HA	1.96	0.81
2:D:24:GLU:O	2:D:45:ILE:HG22	1.82	0.80
2:C:101:GLY:O	2:C:121:PRO:HB3	1.82	0.79
2:D:48:ARG:H	2:D:48:ARG:HD3	1.47	0.79
1:B:164:LYS:HE3	1:B:235:PHE:CE1	2.17	0.78
1:B:149:ASN:C	1:B:151:SER:H	1.92	0.78
1:A:218:HIS:HE1	1:A:230:THR:H	1.33	0.77
1:A:149:ASN:C	1:A:151:SER:H	1.91	0.76
1:A:231:ASN:HD22	1:A:325:ASP:HB3	1.50	0.76
1:A:218:HIS:CE1	1:A:230:THR:H	2.04	0.75
1:A:164:LYS:HE3	1:A:235:PHE:CE1	2.22	0.74
1:B:255:ILE:HB	1:B:275:VAL:HB	1.68	0.74
1:B:218:HIS:CE1	1:B:230:THR:H	2.05	0.74
2:C:97:TYR:HA	2:C:126:VAL:HG23	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PHE:CZ	1:A:278:ASN:HB2	2.22	0.74
2:C:100:ILE:CD1	2:C:122:ILE:H	2.01	0.74
2:D:40:LEU:HB2	2:D:59:ALA:HB2	1.68	0.74
1:B:231:ASN:HD22	1:B:325:ASP:HB3	1.52	0.74
1:B:218:HIS:HE1	1:B:230:THR:H	1.35	0.74
2:C:100:ILE:HD11	2:C:122:ILE:N	2.03	0.74
1:A:191:ILE:HG22	1:A:192:ASN:N	2.02	0.73
1:B:191:ILE:HG22	1:B:192:ASN:N	2.02	0.73
2:D:37:ILE:HD13	2:D:61:TYR:CD1	2.24	0.73
1:A:231:ASN:ND2	1:A:325:ASP:HB3	2.04	0.73
1:A:255:ILE:HB	1:A:275:VAL:HB	1.71	0.73
2:D:25:ARG:HB2	2:D:45:ILE:HG23	1.70	0.72
2:D:10:MET:HG2	2:D:28:TYR:HB3	1.70	0.72
1:B:244:PHE:CZ	1:B:278:ASN:HB2	2.24	0.72
2:D:100:ILE:HG23	2:D:100:ILE:O	1.88	0.72
2:C:100:ILE:CD1	2:C:101:GLY:H	2.04	0.71
1:B:231:ASN:ND2	1:B:325:ASP:HB3	2.05	0.71
2:D:88:GLN:HE21	2:D:106:TYR:HE2	1.38	0.70
2:D:22:ILE:HD12	2:D:22:ILE:H	1.58	0.69
1:B:278:ASN:HB3	1:B:289:CYS:N	2.08	0.69
2:D:98:TYR:HE2	2:D:124:GLU:HB3	1.58	0.69
2:D:88:GLN:OE1	3:F:1:NAG:H5	1.92	0.69
2:D:110:LYS:HG3	2:D:115:ILE:HD11	1.74	0.68
1:A:278:ASN:HB3	1:A:289:CYS:N	2.07	0.68
2:D:35:PHE:CE2	2:D:37:ILE:HD11	2.28	0.68
2:D:11:GLU:HG3	2:D:31:LYS:HG2	1.74	0.68
2:C:22:ILE:HD12	2:C:22:ILE:H	1.57	0.68
2:D:37:ILE:HD13	2:D:61:TYR:HD1	1.57	0.67
2:C:124:GLU:HG3	2:C:125:LYS:HD3	1.76	0.66
1:A:172:PHE:CE1	1:A:315:PRO:HB3	2.30	0.66
1:B:146:GLN:NE2	1:B:152:GLU:HA	2.09	0.66
1:B:172:PHE:CE1	1:B:315:PRO:HB3	2.31	0.66
2:D:122:ILE:HG22	2:D:123:CYS:N	2.11	0.65
2:C:49:ASN:O	2:C:51:THR:N	2.30	0.65
2:C:125:LYS:HD3	2:C:125:LYS:H	1.62	0.64
1:A:169:VAL:HG23	1:A:322:ARG:HB3	1.80	0.64
1:B:153:SER:O	1:B:154:ASN:C	2.40	0.64
2:C:49:ASN:N	2:C:49:ASN:OD1	2.31	0.64
2:D:121:PRO:C	2:D:122:ILE:HD12	2.23	0.64
3:F:2:NAG:H3	3:F:2:NAG:C8	2.20	0.64
2:D:48:ARG:O	2:D:50:HIS:N	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:CYS:H1	2:C:50:HIS:HB3	1.61	0.63
1:B:149:ASN:C	1:B:151:SER:N	2.56	0.63
2:D:98:TYR:CE2	2:D:124:GLU:HB3	2.34	0.63
1:B:164:LYS:NZ	1:B:234:GLY:HA3	2.14	0.63
1:B:191:ILE:CG2	1:B:192:ASN:N	2.61	0.63
1:B:305:GLN:HG3	1:B:306:THR:H	1.63	0.62
2:C:100:ILE:HD13	2:C:101:GLY:H	1.63	0.62
1:A:191:ILE:CG2	1:A:192:ASN:N	2.62	0.62
2:D:36:TYR:C	2:D:37:ILE:HD12	2.24	0.62
1:A:278:ASN:HA	1:A:289:CYS:HB2	1.81	0.62
2:D:49:ASN:O	2:D:50:HIS:HB2	1.99	0.62
1:A:305:GLN:HG3	1:A:306:THR:H	1.65	0.61
2:D:48:ARG:HD3	2:D:48:ARG:N	2.13	0.61
1:B:169:VAL:HG23	1:B:322:ARG:HB3	1.83	0.61
1:B:282:ILE:HG23	2:D:29:LYS:HB2	1.83	0.61
1:A:164:LYS:NZ	1:A:234:GLY:HA3	2.16	0.61
2:D:62:ARG:HG3	2:D:85:PHE:CZ	2.35	0.61
2:C:88:GLN:OE1	3:E:1:NAG:H5	2.01	0.60
1:A:279:ARG:HH11	1:A:279:ARG:HG3	1.66	0.60
2:C:71:PRO:O	2:C:72:LEU:C	2.45	0.60
1:A:148:MET:HE2	1:A:182:PHE:HB2	1.83	0.60
2:C:126:VAL:OXT	2:C:126:VAL:HG12	2.02	0.60
1:A:278:ASN:O	1:A:278:ASN:ND2	2.33	0.59
2:D:12:LEU:HD12	2:D:27:ASP:O	2.01	0.59
2:C:12:LEU:HD11	2:C:26:VAL:CG2	2.30	0.59
1:B:148:MET:HE2	1:B:182:PHE:HB2	1.83	0.59
1:B:278:ASN:HA	1:B:289:CYS:HB2	1.84	0.59
1:B:276:MET:HE2	1:B:291:ARG:HH11	1.68	0.59
1:B:261:TYR:O	1:B:261:TYR:CD2	2.56	0.59
1:B:279:ARG:HG3	1:B:279:ARG:HH11	1.68	0.59
1:A:192:ASN:HB2	1:A:295:SER:HB3	1.85	0.58
2:D:75:GLN:HE21	2:D:92:ILE:HD12	1.68	0.58
2:C:104:ILE:O	2:C:105:LEU:HD23	2.04	0.58
2:C:125:LYS:O	2:C:126:VAL:HB	2.03	0.58
1:A:191:ILE:CG2	1:A:192:ASN:H	2.16	0.58
2:D:88:GLN:NE2	2:D:106:TYR:HE2	2.00	0.58
1:B:191:ILE:CG2	1:B:192:ASN:H	2.17	0.58
2:C:61:TYR:N	2:C:61:TYR:CD1	2.72	0.58
1:B:192:ASN:HB2	1:B:295:SER:HB3	1.86	0.57
1:A:164:LYS:HZ3	1:A:234:GLY:HA3	1.70	0.57
1:A:172:PHE:CZ	1:A:315:PRO:HB3	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:PHE:CE2	2:C:37:ILE:HD11	2.39	0.57
2:D:47:ASP:O	2:D:48:ARG:C	2.47	0.57
2:C:121:PRO:O	2:C:122:ILE:HD13	2.04	0.57
1:B:264:SER:C	1:B:266:ARG:H	2.13	0.57
2:D:88:GLN:NE2	2:D:106:TYR:CE2	2.68	0.57
2:D:100:ILE:HG22	2:D:122:ILE:O	2.03	0.57
1:A:276:MET:HE2	1:A:291:ARG:HH11	1.70	0.56
1:B:278:ASN:O	1:B:278:ASN:ND2	2.30	0.56
1:A:264:SER:C	1:A:266:ARG:H	2.12	0.56
1:B:168:LEU:CD2	1:B:321:ILE:HD13	2.35	0.56
2:C:103:GLU:OE1	2:C:103:GLU:N	2.34	0.56
1:A:140:PRO:HD2	1:A:157:LYS:HD3	1.88	0.56
2:D:2:GLU:HA	2:D:18:PRO:O	2.06	0.56
1:A:168:LEU:CD2	1:A:321:ILE:HD13	2.35	0.56
1:B:265:ASP:OD1	1:B:267:THR:OG1	2.23	0.56
2:C:4:PRO:HG3	2:C:52:TRP:CZ2	2.41	0.55
2:C:124:GLU:CG	2:C:125:LYS:HD3	2.36	0.55
2:C:101:GLY:O	2:C:102:GLU:C	2.49	0.55
2:C:32:LYS:HD3	2:C:111:GLY:O	2.07	0.55
2:D:10:MET:HG2	2:D:28:TYR:CB	2.37	0.55
1:A:209:LEU:HD21	2:C:13:ILE:HD13	1.89	0.55
2:C:4:PRO:HG2	2:C:26:VAL:HG21	1.89	0.55
1:A:183:ASN:OD1	1:A:310:THR:HA	2.06	0.55
2:D:104:ILE:O	2:D:105:LEU:HD23	2.07	0.54
1:B:172:PHE:CZ	1:B:315:PRO:HB3	2.42	0.54
2:D:25:ARG:CB	2:D:45:ILE:HG23	2.37	0.54
2:D:113:VAL:HG12	2:D:115:ILE:HG23	1.88	0.54
2:C:22:ILE:HD12	2:C:22:ILE:N	2.22	0.54
2:C:113:VAL:HG12	2:C:115:ILE:HG23	1.90	0.54
1:A:265:ASP:OD1	1:A:267:THR:OG1	2.26	0.54
1:B:164:LYS:HZ3	1:B:234:GLY:HA3	1.70	0.54
1:B:183:ASN:OD1	1:B:310:THR:HA	2.09	0.53
1:B:186:THR:HG22	1:B:311:LEU:HD13	1.89	0.53
2:C:92:ILE:HG12	2:C:92:ILE:O	2.07	0.53
1:A:133:THR:O	1:A:218:HIS:HA	2.08	0.53
1:B:133:THR:O	1:B:218:HIS:HA	2.09	0.53
1:B:140:PRO:HD2	1:B:157:LYS:HD3	1.91	0.53
2:C:88:GLN:NE2	2:C:106:TYR:CE2	2.77	0.52
2:C:98:TYR:CD1	2:C:126:VAL:HG22	2.43	0.52
2:C:100:ILE:CD1	2:C:101:GLY:N	2.73	0.52
1:B:274:SER:HB2	1:B:293:THR:HG23	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:GLY:O	2:D:126:VAL:HG22	2.09	0.52
2:D:98:TYR:HE2	2:D:124:GLU:CB	2.22	0.52
2:C:97:TYR:HA	2:C:126:VAL:CG2	2.39	0.52
1:A:274:SER:HB2	1:A:293:THR:HG23	1.91	0.52
1:A:186:THR:HG22	1:A:311:LEU:HD13	1.90	0.52
2:C:37:ILE:HD13	2:C:61:TYR:CD1	2.45	0.51
2:D:97:TYR:N	2:D:97:TYR:CD1	2.78	0.51
2:C:98:TYR:HD1	2:C:126:VAL:CG2	2.24	0.51
1:B:174:TYR:HA	5:B:8:HOH:O	2.10	0.51
2:C:98:TYR:HD1	2:C:126:VAL:HG22	1.76	0.51
2:D:22:ILE:HD12	2:D:22:ILE:N	2.25	0.51
2:C:110:LYS:HG3	2:C:115:ILE:HD11	1.92	0.51
2:D:24:GLU:C	2:D:45:ILE:HG22	2.34	0.51
2:D:47:ASP:C	2:D:47:ASP:OD2	2.54	0.51
1:A:136:THR:HB	5:A:1:HOH:O	2.11	0.51
1:A:278:ASN:HD22	1:A:278:ASN:C	2.19	0.50
1:A:191:ILE:HG22	1:A:192:ASN:H	1.73	0.50
2:C:101:GLY:C	2:C:102:GLU:O	2.53	0.50
1:B:261:TYR:OH	1:B:303:GLU:CG	2.59	0.50
2:D:48:ARG:C	2:D:50:HIS:N	2.69	0.50
2:C:100:ILE:HD11	2:C:122:ILE:HB	1.93	0.50
2:C:35:PHE:O	2:C:60:CYS:HA	2.11	0.50
2:C:65:CYS:HB3	2:C:116:TRP:NE1	2.27	0.50
2:D:77:VAL:HG23	2:D:77:VAL:O	2.11	0.50
1:B:168:LEU:HD23	1:B:321:ILE:HD13	1.94	0.49
2:C:1:CYS:HA	2:C:50:HIS:O	2.11	0.49
2:C:59:ALA:HB3	5:C:3083:HOH:O	2.11	0.49
1:A:168:LEU:HD23	1:A:321:ILE:HD13	1.94	0.49
1:B:278:ASN:HD22	1:B:278:ASN:C	2.18	0.49
1:A:138:VAL:O	1:A:139:ASN:C	2.56	0.49
2:C:2:GLU:O	2:C:3:GLU:C	2.56	0.49
2:D:122:ILE:HD12	2:D:122:ILE:N	2.27	0.49
1:B:207:THR:HG22	1:B:213:LYS:C	2.38	0.49
2:D:48:ARG:C	2:D:50:HIS:H	2.21	0.49
1:A:153:SER:O	1:A:154:ASN:C	2.55	0.48
2:C:7:PHE:HZ	2:C:55:VAL:HG13	1.77	0.48
2:C:75:GLN:HE21	2:C:77:VAL:HG11	1.77	0.48
2:D:11:GLU:OE1	2:D:31:LYS:HD3	2.13	0.48
2:D:90:HIS:CD2	2:D:104:ILE:HG12	2.47	0.48
1:B:144:ASN:HB2	1:B:214:THR:CG2	2.43	0.48
2:D:7:PHE:CD2	2:D:10:MET:HE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:TYR:O	2:C:108:GLU:HG3	2.14	0.48
2:D:37:ILE:HD12	2:D:37:ILE:N	2.28	0.48
2:C:62:ARG:HB3	2:C:85:PHE:CE2	2.48	0.48
1:A:276:MET:HE2	1:A:291:ARG:NH1	2.29	0.48
1:B:276:MET:HE2	1:B:291:ARG:NH1	2.29	0.48
2:D:24:GLU:O	2:D:45:ILE:CG2	2.59	0.47
2:D:59:ALA:HB3	5:D:3085:HOH:O	2.13	0.47
1:A:282:ILE:HG23	2:C:29:LYS:HB2	1.96	0.47
1:B:143:ALA:HB1	1:B:156:CYS:O	2.13	0.47
2:D:122:ILE:CG2	2:D:123:CYS:N	2.76	0.47
1:A:148:MET:O	1:A:151:SER:HB2	2.14	0.47
2:C:124:GLU:CG	2:C:125:LYS:H	2.27	0.47
1:B:138:VAL:O	1:B:139:ASN:C	2.56	0.47
1:B:152:GLU:HG3	1:B:153:SER:H	1.79	0.47
1:A:149:ASN:C	1:A:151:SER:N	2.59	0.47
1:A:157:LYS:HB3	1:A:176:ILE:HB	1.97	0.47
2:D:68:ILE:HB	2:D:89:MET:HE3	1.96	0.47
2:C:122:ILE:HG22	2:C:123:CYS:N	2.30	0.47
1:A:143:ALA:HB1	1:A:156:CYS:O	2.14	0.47
1:A:144:ASN:HB2	1:A:214:THR:CG2	2.45	0.47
1:A:192:ASN:HA	1:A:294:TRP:O	2.15	0.46
1:B:269:PHE:CG	1:B:302:PRO:HB3	2.50	0.46
2:D:110:LYS:CG	2:D:115:ILE:HD11	2.41	0.46
2:D:22:ILE:H	2:D:22:ILE:CD1	2.26	0.46
2:D:100:ILE:HG22	2:D:122:ILE:H	1.79	0.46
1:A:269:PHE:CG	1:A:302:PRO:HB3	2.50	0.46
1:A:276:MET:CE	1:A:291:ARG:NH1	2.79	0.46
2:D:12:LEU:HD12	2:D:13:ILE:H	1.80	0.46
1:B:149:ASN:O	1:B:151:SER:N	2.49	0.46
1:B:192:ASN:HA	1:B:294:TRP:O	2.15	0.46
2:C:22:ILE:H	2:C:22:ILE:CD1	2.27	0.46
2:C:61:TYR:N	2:C:61:TYR:HD1	2.12	0.46
2:C:78:PRO:O	2:C:79:ALA:C	2.57	0.46
2:C:100:ILE:HD11	2:C:122:ILE:CA	2.44	0.46
2:D:75:GLN:NE2	2:D:92:ILE:HD12	2.30	0.46
2:C:92:ILE:HD13	2:C:92:ILE:H	1.79	0.46
2:C:97:TYR:N	2:C:97:TYR:CD1	2.83	0.46
2:D:78:PRO:O	2:D:79:ALA:C	2.57	0.46
1:B:232:ALA:O	1:B:233:LYS:C	2.58	0.46
1:A:149:ASN:O	1:A:151:SER:N	2.49	0.46
1:A:173:VAL:HG22	1:A:174:TYR:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLU:HG3	1:B:324:ASP:N	2.31	0.46
2:C:105:LEU:HD11	2:C:119:LYS:C	2.40	0.46
1:B:191:ILE:HG22	1:B:192:ASN:H	1.75	0.46
2:D:11:GLU:HG3	2:D:31:LYS:HE3	1.96	0.46
1:A:202:THR:HG22	1:A:202:THR:O	2.16	0.45
2:C:113:VAL:CG1	2:C:115:ILE:HG23	2.46	0.45
1:A:152:GLU:O	1:A:153:SER:CB	2.65	0.45
1:A:310:THR:HG22	1:A:311:LEU:N	2.32	0.45
2:C:75:GLN:HB3	2:C:92:ILE:HD11	1.99	0.45
1:A:140:PRO:HD2	1:A:157:LYS:CD	2.46	0.45
1:B:276:MET:HE3	1:B:279:ARG:HB3	1.99	0.45
2:C:89:MET:HB2	2:C:116:TRP:CH2	2.52	0.45
1:A:191:ILE:O	1:A:192:ASN:HB3	2.16	0.45
1:B:276:MET:CE	1:B:291:ARG:NH1	2.79	0.45
2:C:75:GLN:HG2	2:C:77:VAL:HG13	1.98	0.45
2:C:99:LEU:CD1	2:C:103:GLU:CB	2.85	0.45
2:D:19:TYR:HE2	2:D:21:GLU:OE1	2.00	0.45
2:D:48:ARG:O	2:D:49:ASN:C	2.60	0.45
1:A:323:GLU:HG3	1:A:324:ASP:N	2.32	0.45
1:B:276:MET:HE2	5:B:14:HOH:O	2.16	0.45
2:C:100:ILE:HD12	2:C:101:GLY:N	2.31	0.45
2:C:122:ILE:CG2	2:C:123:CYS:N	2.79	0.45
1:A:209:LEU:HD21	2:C:13:ILE:CD1	2.47	0.45
1:A:232:ALA:O	1:A:233:LYS:C	2.59	0.45
1:B:206:LEU:HD12	1:B:206:LEU:HA	1.78	0.45
2:D:48:ARG:H	2:D:48:ARG:HD2	1.77	0.45
1:A:130:ASN:HD22	1:A:219:LYS:HD3	1.82	0.44
1:A:207:THR:HG22	1:A:213:LYS:C	2.41	0.44
1:B:191:ILE:O	1:B:192:ASN:HB3	2.17	0.44
1:A:304:VAL:O	1:A:305:GLN:C	2.60	0.44
1:B:173:VAL:HG22	1:B:174:TYR:N	2.31	0.44
2:C:10:MET:CG	2:C:28:TYR:HB3	2.47	0.44
2:D:99:LEU:HD21	2:D:103:GLU:HA	1.99	0.44
1:B:236:MET:HB3	1:B:288:TYR:CD2	2.52	0.44
1:B:310:THR:HG22	1:B:312:VAL:HG23	1.99	0.44
2:C:31:LYS:HB3	2:C:31:LYS:NZ	2.32	0.44
2:D:1:CYS:SG	2:D:46:CYS:HB2	2.46	0.44
2:D:70:ASP:C	2:D:71:PRO:O	2.61	0.44
2:D:100:ILE:O	2:D:100:ILE:CG2	2.60	0.44
1:A:279:ARG:HG3	1:A:279:ARG:NH1	2.33	0.44
2:D:65:CYS:HB3	2:D:116:TRP:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:HB3	1:B:176:ILE:HB	1.98	0.44
2:D:106:TYR:HB2	2:D:117:SER:HB3	2.00	0.43
2:C:37:ILE:HG22	2:C:38:PRO:O	2.17	0.43
1:A:236:MET:HB3	1:A:288:TYR:CD2	2.54	0.43
1:A:310:THR:HG22	1:A:312:VAL:HG23	1.99	0.43
1:B:140:PRO:HD2	1:B:157:LYS:CD	2.48	0.43
1:A:152:GLU:O	1:A:153:SER:OG	2.34	0.43
1:B:152:GLU:HG3	1:B:153:SER:N	2.33	0.43
1:B:152:GLU:O	1:B:153:SER:OG	2.36	0.43
2:D:122:ILE:HG22	2:D:123:CYS:H	1.82	0.43
1:B:310:THR:HG22	1:B:311:LEU:N	2.32	0.43
2:D:56:SER:OG	2:D:57:ASP:N	2.52	0.43
2:D:35:PHE:CD2	2:D:37:ILE:HD11	2.53	0.43
2:C:98:TYR:HE1	2:C:126:VAL:H	1.67	0.43
2:D:19:TYR:HE1	5:D:3084:HOH:O	2.01	0.43
1:A:153:SER:O	1:A:153:SER:OG	2.37	0.42
1:B:291:ARG:NH1	5:B:14:HOH:O	2.46	0.42
1:A:171:ALA:O	1:A:317:THR:HA	2.19	0.42
2:C:67:TYR:HA	2:C:83:TYR:CE2	2.54	0.42
2:D:11:GLU:HG3	2:D:31:LYS:CG	2.46	0.42
1:B:171:ALA:O	1:B:317:THR:HA	2.19	0.42
2:D:40:LEU:CB	2:D:59:ALA:HB2	2.43	0.42
2:D:104:ILE:HG22	2:D:105:LEU:N	2.33	0.42
1:A:276:MET:HE3	1:A:279:ARG:HB3	2.02	0.42
2:D:96:GLY:C	2:D:97:TYR:CD1	2.98	0.42
1:B:264:SER:C	1:B:266:ARG:N	2.78	0.42
2:C:11:GLU:HG2	2:C:31:LYS:HG2	2.01	0.42
2:D:62:ARG:HG3	2:D:85:PHE:CD2	2.51	0.42
2:C:35:PHE:HE2	2:C:37:ILE:HD11	1.84	0.42
1:B:164:LYS:HE3	1:B:235:PHE:CD1	2.54	0.42
2:D:72:LEU:O	2:D:73:ASN:HB2	2.20	0.42
1:A:174:TYR:HE2	1:A:176:ILE:HD11	1.85	0.41
1:B:135:TRP:CD1	1:B:135:TRP:C	2.97	0.41
1:A:305:GLN:HG3	1:A:306:THR:N	2.34	0.41
1:B:174:TYR:HE2	1:B:176:ILE:HD11	1.85	0.41
1:B:202:THR:HG22	1:B:202:THR:O	2.19	0.41
2:C:88:GLN:NE2	2:C:106:TYR:CD2	2.88	0.41
2:D:78:PRO:HB2	2:D:81:GLY:HA2	2.02	0.41
1:B:146:GLN:HE21	1:B:152:GLU:HA	1.85	0.41
2:C:1:CYS:SG	2:C:50:HIS:C	3.03	0.41
2:C:99:LEU:HD22	2:C:103:GLU:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:ILE:HG22	2:D:38:PRO:O	2.20	0.41
1:B:304:VAL:O	1:B:305:GLN:C	2.63	0.41
2:C:12:LEU:HD12	2:C:27:ASP:O	2.21	0.41
2:C:89:MET:HB2	2:C:116:TRP:CZ3	2.56	0.41
2:C:126:VAL:OXT	2:C:126:VAL:CG1	2.68	0.41
1:A:269:PHE:CD1	1:A:302:PRO:HB3	2.55	0.41
1:A:264:SER:C	1:A:266:ARG:N	2.77	0.41
1:A:135:TRP:CD1	1:A:135:TRP:C	2.96	0.41
1:A:194:THR:OG1	1:A:293:THR:HB	2.21	0.41
1:B:194:THR:OG1	1:B:293:THR:HB	2.20	0.41
2:C:9:ALA:HB1	2:C:34:TYR:CD2	2.56	0.41
2:C:75:GLN:HE21	2:C:77:VAL:CG1	2.33	0.41
2:D:1:CYS:N	2:D:20:TYR:O	2.54	0.41
1:B:261:TYR:OH	1:B:303:GLU:HG3	2.20	0.41
1:B:305:GLN:HG3	1:B:306:THR:N	2.32	0.41
2:D:70:ASP:O	2:D:71:PRO:C	2.61	0.41
1:A:190:ASN:OD1	1:A:297:ASN:HB2	2.20	0.41
1:A:198:PHE:HB3	1:A:286:THR:HG22	2.03	0.41
1:B:261:TYR:OH	1:B:303:GLU:HG2	2.21	0.41
2:D:52:TRP:O	2:D:53:LEU:C	2.63	0.41
1:B:130:ASN:HD22	1:B:219:LYS:HD3	1.85	0.40
2:C:99:LEU:HD13	2:C:103:GLU:HB3	1.96	0.40
2:D:47:ASP:O	2:D:47:ASP:OD2	2.39	0.40
1:A:161:THR:HB	1:A:172:PHE:HB3	2.02	0.40
2:C:91:PHE:CD2	2:C:121:PRO:HD2	2.57	0.40
2:D:97:TYR:HA	2:D:126:VAL:HG13	2.02	0.40
1:B:147:ILE:HD13	1:B:193:PHE:HD2	1.85	0.40
1:A:147:ILE:HD11	1:A:195:ALA:HB2	2.03	0.40
2:C:37:ILE:HD13	2:C:61:TYR:CG	2.57	0.40
2:D:7:PHE:HB2	2:D:10:MET:HB3	2.03	0.40
2:D:90:HIS:NE2	2:D:104:ILE:HD13	2.37	0.40

All (2) 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)
1:A:319:TYR:OH	1:A:319:TYR:OH[2_665]	1.90	0.30
1:B:319:TYR:OH	1:B:319:TYR:OH[3_555]	1.90	0.30

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	195/197 (99%)	173 (89%)	13 (7%)	9 (5%)	2	3
1	B	195/197 (99%)	173 (89%)	13 (7%)	9 (5%)	2	3
2	C	124/126 (98%)	107 (86%)	13 (10%)	4 (3%)	3	7
2	D	124/126 (98%)	106 (86%)	14 (11%)	4 (3%)	3	7
All	All	638/646 (99%)	559 (88%)	53 (8%)	26 (4%)	2	4

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
2	C	102	GLU
1	A	278	ASN
1	B	154	ASN
1	B	278	ASN
2	D	2	GLU
2	D	49	ASN
1	A	150	SER
1	A	305	GLN
1	B	150	SER
1	B	305	GLN
1	A	192	ASN
1	A	215	PRO
1	A	265	ASP
1	B	192	ASN
1	B	215	PRO
1	B	265	ASP
2	C	72	LEU
1	A	139	ASN
1	A	309	THR
1	B	139	ASN
1	B	309	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	3	GLU
2	C	101	GLY
2	D	53	LEU
2	C	100	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/175 (100%)	160 (91%)	15 (9%)	10	21
1	B	175/175 (100%)	160 (91%)	15 (9%)	10	21
2	C	110/110 (100%)	98 (89%)	12 (11%)	6	12
2	D	110/110 (100%)	98 (89%)	12 (11%)	6	12
All	All	570/570 (100%)	516 (90%)	54 (10%)	8	17

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ILE
1	A	150	SER
1	A	151	SER
1	A	152	GLU
1	A	155	ASP
1	A	206	LEU
1	A	207	THR
1	A	214	THR
1	A	262	THR
1	A	267	THR
1	A	278	ASN
1	A	282	ILE
1	A	292	ILE
1	A	293	THR
1	A	305	GLN
1	B	147	ILE
1	B	150	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	151	SER
1	B	154	ASN
1	B	155	ASP
1	B	206	LEU
1	B	207	THR
1	B	214	THR
1	B	262	THR
1	B	267	THR
1	B	278	ASN
1	B	282	ILE
1	B	292	ILE
1	B	293	THR
1	B	305	GLN
2	C	21	GLU
2	C	37	ILE
2	C	39	PRO
2	C	40	LEU
2	C	49	ASN
2	C	61	TYR
2	C	88	GLN
2	C	92	ILE
2	C	100	ILE
2	C	103	GLU
2	C	113	VAL
2	C	125	LYS
2	D	17	LYS
2	D	21	GLU
2	D	39	PRO
2	D	40	LEU
2	D	45	ILE
2	D	48	ARG
2	D	51	THR
2	D	75	GLN
2	D	92	ILE
2	D	97	TYR
2	D	98	TYR
2	D	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	ASN
1	A	180	ASN
1	A	218	HIS
1	A	223	ASN
1	A	231	ASN
1	A	305	GLN
1	B	146	GLN
1	B	149	ASN
1	B	180	ASN
1	B	218	HIS
1	B	231	ASN
1	B	305	GLN
2	C	75	GLN
2	C	94	ASN
2	D	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	E	1	2,3	14,14,15	0.66	0	17,19,21	1.21	4 (23%)
3	NAG	E	2	3	14,14,15	0.52	0	17,19,21	0.73	0
3	BMA	E	3	3	11,11,12	0.50	0	15,15,17	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	2,3	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
3	NAG	F	2	3	14,14,15	0.73	0	17,19,21	1.39	2 (11%)
3	BMA	F	3	3	11,11,12	0.47	0	15,15,17	1.02	2 (13%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C4-C3-C2	4.31	117.34	111.02
3	E	1	NAG	C3-C4-C5	2.55	114.86	110.23
3	F	1	NAG	C2-N2-C7	-2.47	119.60	122.90
3	F	3	BMA	C1-C2-C3	2.42	113.17	109.64
3	F	3	BMA	C1-O5-C5	2.42	115.43	112.19
3	E	3	BMA	C1-C2-C3	2.37	113.09	109.64
3	E	1	NAG	O5-C1-C2	-2.29	107.75	111.29
3	E	1	NAG	C4-C3-C2	2.07	114.05	111.02
3	F	2	NAG	C2-N2-C7	-2.05	120.15	122.90
3	E	1	NAG	C2-N2-C7	-2.03	120.17	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

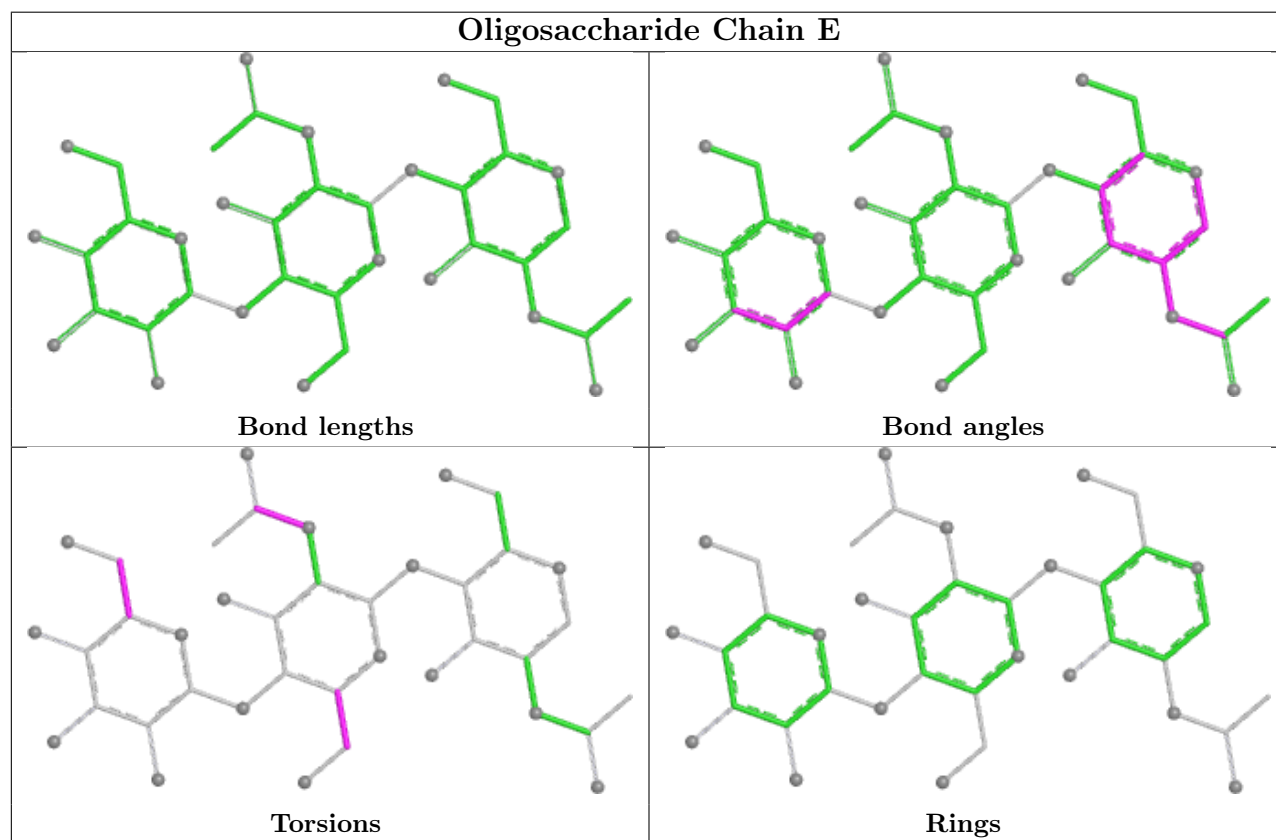
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	3	BMA	O5-C5-C6-O6

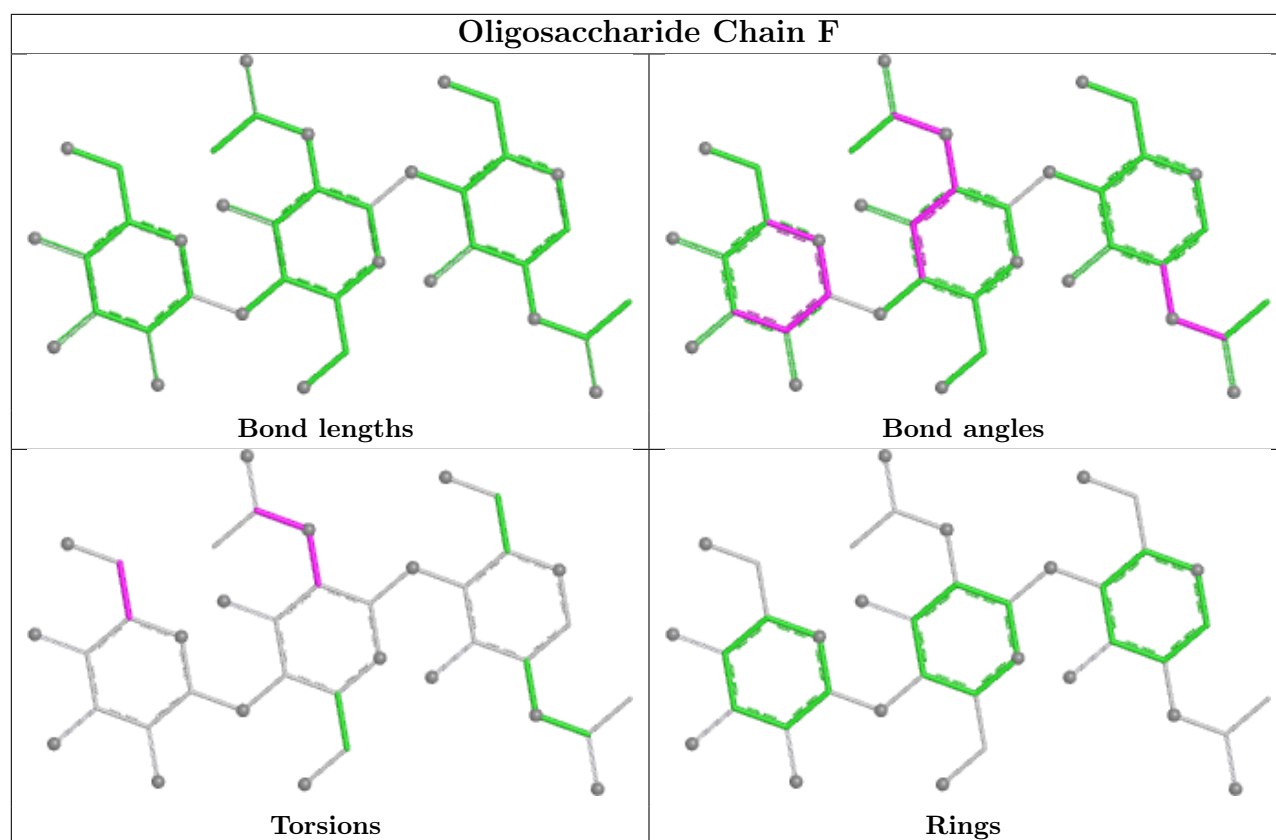
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	E	1	NAG	1	0
3	F	2	NAG	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 [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	197/197 (100%)	-1.69	0 100 100	27, 39, 60, 75	0
1	B	197/197 (100%)	-1.69	0 100 100	23, 38, 60, 75	0
2	C	126/126 (100%)	-1.69	0 100 100	34, 52, 71, 78	0
2	D	126/126 (100%)	-1.71	0 100 100	26, 52, 74, 83	0
All	All	646/646 (100%)	-1.70	0 100 100	23, 44, 68, 83	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

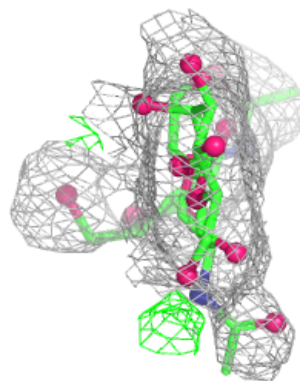
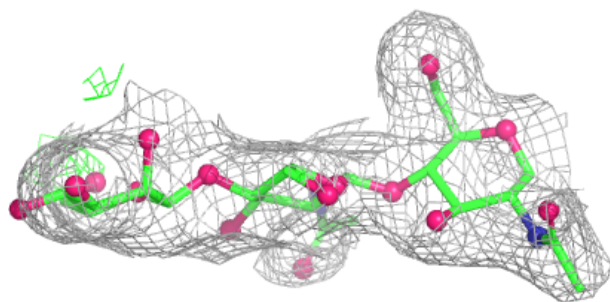
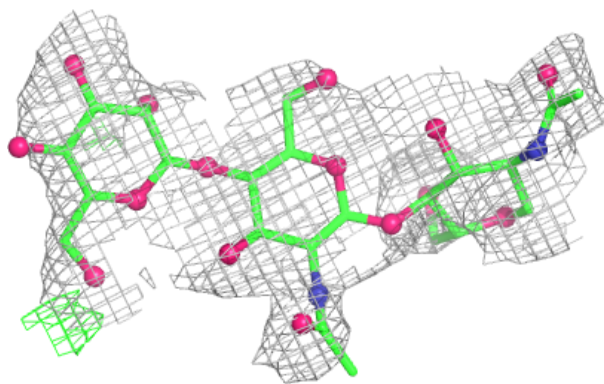
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	E	3	11/12	0.97	0.05	95,97,97,97	0
3	NAG	F	2	14/15	0.97	0.04	87,92,95,96	0
3	BMA	F	3	11/12	0.97	0.04	98,99,100,100	0
3	NAG	F	1	14/15	0.99	0.04	67,73,77,83	0
3	NAG	E	2	14/15	0.99	0.04	84,88,90,93	0
3	NAG	E	1	14/15	0.99	0.03	68,72,75,80	0

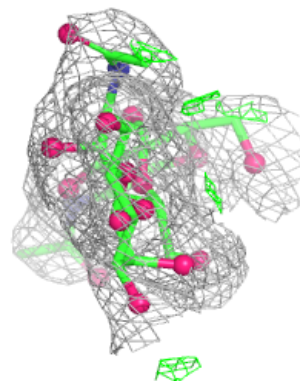
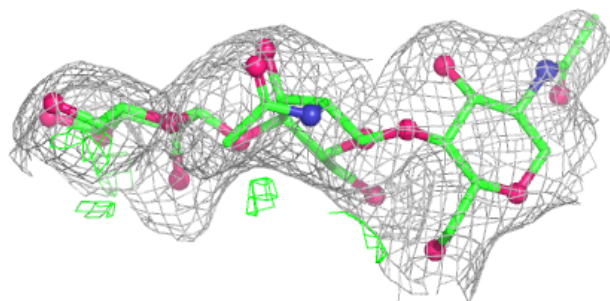
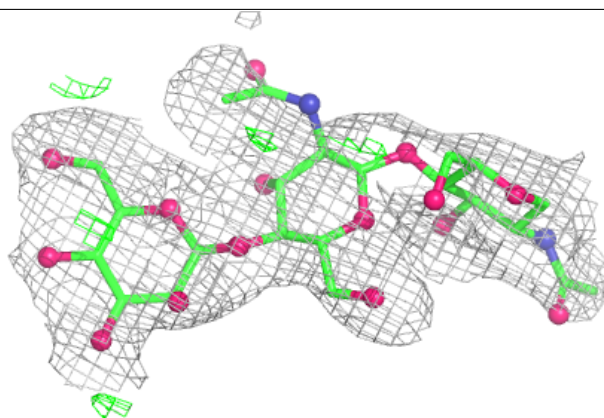
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	D	3082	1/1	0.99	0.03	67,67,67,67	0
4	CA	D	3081	1/1	1.00	0.02	53,53,53,53	0
4	CA	C	3081	1/1	1.00	0.03	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.