



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:03 AM UTC

PDB ID : 4CC1 / pdb_00004cc1
Title : Notch ligand, Jagged-1, contains an N-terminal C2 domain
Authors : Chilakuri, C.R.; Sheppard, D.; Ilagan, M.X.G.; Holt, L.R.; Abbott, F.; Liang, S.; Kopan, R.; Handford, P.A.; Lea, S.M.
Deposited on : 2013-10-17
Resolution : 2.84 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

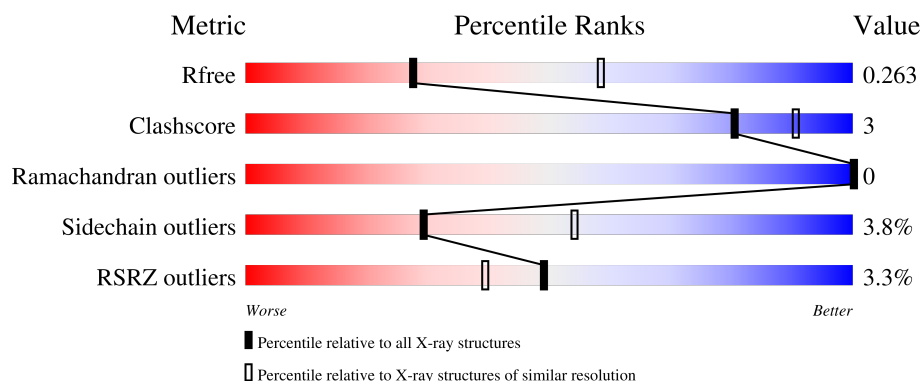
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

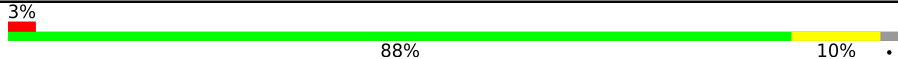
The reported resolution of this entry is 2.84 Å.

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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	312	 3% 88% 10% .
1	B	312	 4% 87% 10% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4798 atoms, of which 12 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN JAGGED-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2363	1448	424	457	34			
1	B	306	Total	C	N	O	S	0	0	0
			2363	1448	424	457	34			

There are 16 discrepancies between the modelled and reference sequences:

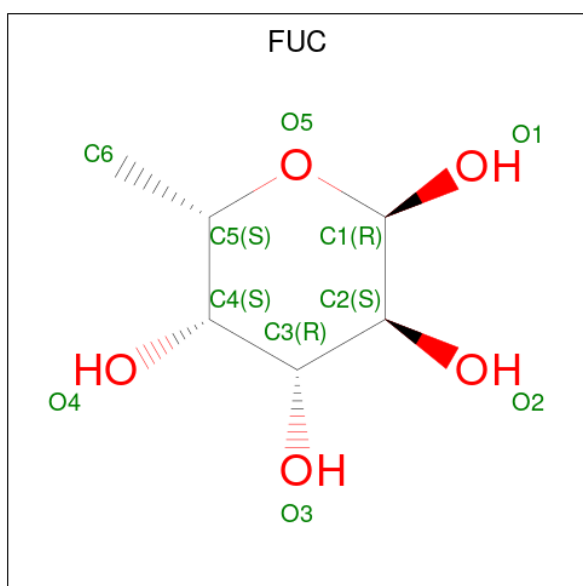
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	-	expression tag	UNP P78504
A	337	ASP	-	expression tag	UNP P78504
A	338	HIS	-	expression tag	UNP P78504
A	339	HIS	-	expression tag	UNP P78504
A	340	HIS	-	expression tag	UNP P78504
A	341	HIS	-	expression tag	UNP P78504
A	342	HIS	-	expression tag	UNP P78504
A	343	HIS	-	expression tag	UNP P78504
B	336	VAL	-	expression tag	UNP P78504
B	337	ASP	-	expression tag	UNP P78504
B	338	HIS	-	expression tag	UNP P78504
B	339	HIS	-	expression tag	UNP P78504
B	340	HIS	-	expression tag	UNP P78504
B	341	HIS	-	expression tag	UNP P78504
B	342	HIS	-	expression tag	UNP P78504
B	343	HIS	-	expression tag	UNP P78504

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

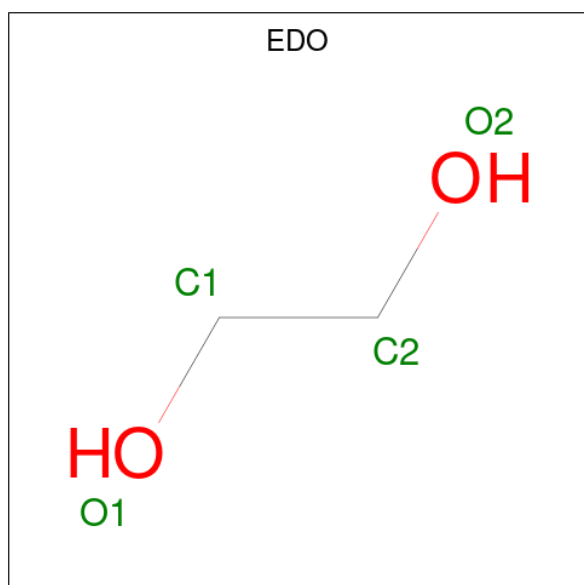
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Cl 4 4	0	0
5	B	2	Total Cl 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C H O 10 2 6 2	0	0
6	B	1	Total C H O 10 2 6 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0

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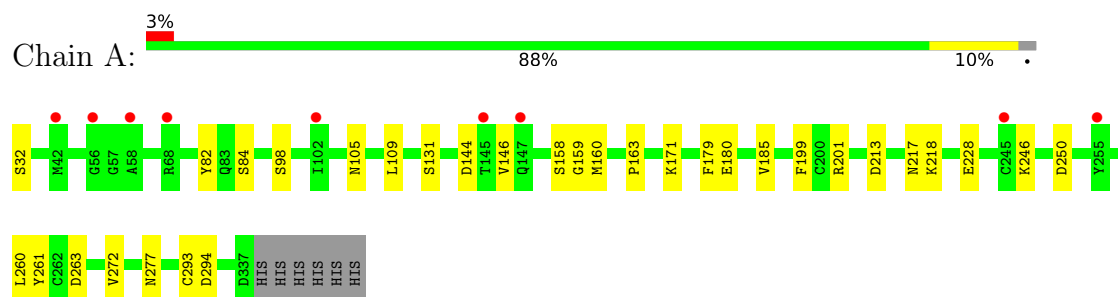
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	5	Total	O	0	0
			5	5		

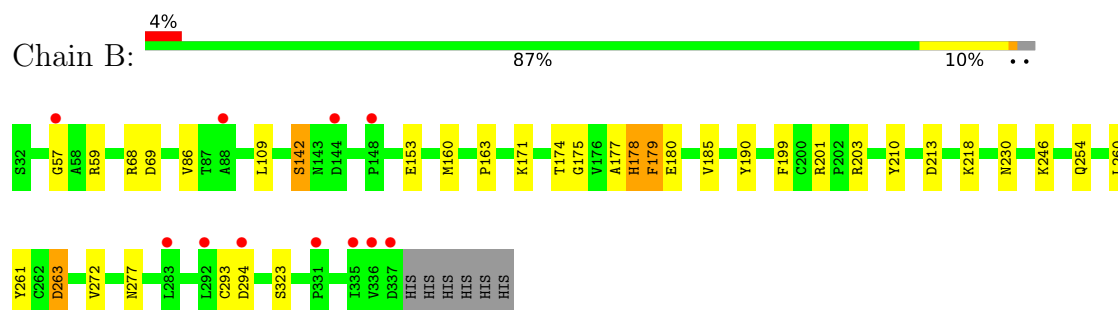
3 Residue-property plots

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: PROTEIN JAGGED-1



• Molecule 1: PROTEIN JAGGED-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.95Å 60.56Å 63.03Å 92.89° 104.95° 105.92°	Depositor
Resolution (Å)	60.38 – 2.84 60.38 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.2 (60.38-2.84) 98.2 (60.38-2.84)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.196 , 0.249 (Not available) , 0.263	Depositor DCC
R_{free} test set	988 reflections (5.59%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4798	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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: CL, FUC, CA, NAG, EDO

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	0.84	1/2425 (0.0%)	1.28	7/3283 (0.2%)
1	B	0.84	1/2425 (0.0%)	1.29	12/3283 (0.4%)
All	All	0.84	2/4850 (0.0%)	1.28	19/6566 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	MET	SD-CE	7.68	1.98	1.79
1	B	178	HIS	CA-C	-5.46	1.46	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ASP	CA-CB-CG	7.61	120.21	112.60
1	A	246	LYS	N-CA-C	-7.28	103.50	113.18
1	B	57	GLY	N-CA-C	7.20	118.29	111.67
1	A	263	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	277	ASN	N-CA-C	-6.99	104.74	113.55
1	B	213	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	277	ASN	N-CA-C	-6.71	105.10	113.55
1	A	294	ASP	CA-CB-CG	6.52	119.12	112.60
1	B	175	GLY	CA-C-N	6.41	128.72	120.70
1	B	175	GLY	C-N-CA	6.41	128.72	120.70
1	B	294	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	250	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	105	ASN	CA-CB-CG	5.78	118.38	112.60
1	B	246	LYS	N-CA-C	-5.58	106.60	113.41
1	B	254	GLN	N-CA-C	-5.32	103.51	110.53
1	A	179	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	179	PHE	CA-CB-CG	5.14	118.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	SER	CA-C-N	5.07	127.96	120.82
1	B	142	SER	C-N-CA	5.07	127.96	120.82

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	2363	0	2145	10	0
1	B	2363	0	2146	14	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	10	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	2	0	0	1	0
6	B	8	12	12	4	0
7	A	1	0	0	1	0
7	B	5	0	0	0	0
All	All	4786	12	4339	24	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 3.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:H	6:B:1342:EDO:H21	1.58	0.69
1:B:180:GLU:HG3	6:B:1341:EDO:H22	1.81	0.63
1:B:260:LEU:HD23	1:B:261:TYR:CZ	2.43	0.53
1:A:260:LEU:HD23	1:A:261:TYR:CZ	2.44	0.52
1:A:272:VAL:O	1:A:293:CYS:HB2	2.12	0.50
1:A:199:PHE:CE1	1:A:201:ARG:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLU:HG3	6:B:1341:EDO:C2	2.43	0.48
1:A:171:LYS:HG2	1:A:180:GLU:HG2	1.96	0.48
1:B:272:VAL:O	1:B:293:CYS:HB2	2.13	0.48
1:A:32:SER:HB3	7:A:2001:HOH:O	2.15	0.47
1:B:68:ARG:HB2	1:B:69:ASP:H	1.55	0.47
1:B:210:TYR:CZ	1:B:218:LYS:HE3	2.50	0.47
1:A:163:PRO:HA	1:A:185:VAL:O	2.15	0.47
1:B:178:HIS:HB3	6:B:1341:EDO:H12	1.95	0.46
1:B:163:PRO:HA	1:B:185:VAL:O	2.15	0.46
1:B:230:ASN:HB2	5:B:1340:CL:CL	2.52	0.46
1:B:171:LYS:HG2	1:B:180:GLU:HG2	1.97	0.45
1:A:82:TYR:CE1	1:A:158:SER:HB3	2.52	0.44
1:B:190:TYR:HB2	1:B:199:PHE:CE1	2.54	0.42
1:A:131:SER:HA	1:A:159:GLY:O	2.20	0.42
1:B:153:GLU:HB2	1:B:177:ALA:HB3	2.03	0.41
1:A:213:ASP:OD2	1:A:217:ASN:HB2	2.21	0.41
1:A:218:LYS:HE2	1:A:228:GLU:OE1	2.21	0.41
1:B:153:GLU:HB3	1:B:179:PHE:HE2	1.87	0.40

There are no symmetry-related clashes.

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	304/312 (97%)	282 (93%)	22 (7%)	0	100	100
1	B	304/312 (97%)	277 (91%)	27 (9%)	0	100	100
All	All	608/624 (97%)	559 (92%)	49 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	163/267 (61%)	158 (97%)	5 (3%)	35	59
1	B	210/267 (79%)	201 (96%)	9 (4%)	26	50
All	All	373/534 (70%)	359 (96%)	14 (4%)	29	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	98	SER
1	A	109	LEU
1	A	144	ASP
1	A	146	VAL
1	B	86	VAL
1	B	109	LEU
1	B	142	SER
1	B	160	MET
1	B	174	THR
1	B	201	ARG
1	B	203	ARG
1	B	263	ASP
1	B	323	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	172	GLN
1	B	157	HIS
1	B	242	HIS

5.3.3 RNA ⓘ

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 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	$\# Z > 2$
6	EDO	B	1341	-	3,3,3	0.92	0	2,2,2	0.39	0
2	NAG	A	1338	1	14,14,15	0.33	0	17,19,21	0.56	0
3	FUC	A	1339	1	10,10,11	0.46	0	14,14,16	0.86	1 (7%)
6	EDO	B	1342	-	3,3,3	1.06	0	2,2,2	0.17	0
2	NAG	B	1338	1	14,14,15	0.44	0	17,19,21	0.75	0

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
6	EDO	B	1341	-	-	1/1/1/1	-
2	NAG	A	1338	1	-	2/6/23/26	0/1/1/1
3	FUC	A	1339	1	-	-	0/1/1/1
6	EDO	B	1342	-	-	1/1/1/1	-
2	NAG	B	1338	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1339	FUC	C1-O5-C5	2.81	119.59	112.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1338	NAG	O5-C5-C6-O6
2	A	1338	NAG	C4-C5-C6-O6
2	B	1338	NAG	C4-C5-C6-O6
2	B	1338	NAG	O5-C5-C6-O6
6	B	1341	EDO	O1-C1-C2-O2
6	B	1342	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1341	EDO	3	0
6	B	1342	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	306/312 (98%)	0.13	9 (2%) 53 44	37, 63, 93, 111	0
1	B	306/312 (98%)	0.30	11 (3%) 46 37	33, 65, 131, 157	0
All	All	612/624 (98%)	0.21	20 (3%) 49 39	33, 64, 110, 157	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	GLY	5.0
1	B	292	LEU	3.3
1	B	337	ASP	2.9
1	B	88	ALA	2.8
1	A	255	TYR	2.7
1	A	68	ARG	2.7
1	A	102	ILE	2.7
1	B	144	ASP	2.7
1	B	336	VAL	2.6
1	B	294	ASP	2.5
1	B	283	LEU	2.4
1	B	331	PRO	2.4
1	A	58	ALA	2.3
1	B	148	PRO	2.2
1	A	145	THR	2.2
1	A	147	GLN	2.2
1	A	42	MET	2.1
1	B	57	GLY	2.1
1	A	245	CYS	2.1
1	B	335	ILE	2.1

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](#)

There are no oligosaccharides in this entry.

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
6	EDO	B	1342	4/4	0.76	0.13	44,48,58,58	0
2	NAG	A	1338	14/15	0.77	0.13	94,97,101,102	0
2	NAG	B	1338	14/15	0.81	0.17	105,107,108,109	0
3	FUC	A	1339	10/11	0.91	0.08	66,70,72,73	0
6	EDO	B	1341	4/4	0.92	0.10	36,50,60,60	0
5	CL	B	1343	1/1	0.92	0.06	51,51,51,51	0
5	CL	B	1340	1/1	0.94	0.20	55,55,55,55	0
4	CA	B	1339	1/1	0.95	0.06	85,85,85,85	0
4	CA	A	1340	1/1	0.96	0.10	82,82,82,82	0
5	CL	A	1342	1/1	0.96	0.11	42,42,42,42	0
5	CL	A	1343	1/1	0.97	0.09	51,51,51,51	0
5	CL	A	1344	1/1	0.97	0.07	49,49,49,49	0
5	CL	A	1341	1/1	0.97	0.21	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.