



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2017 – 12:20 PM EDT

PDB ID : 4XBM
Title : X-ray crystal structure of Notch ligand Delta-like 1
Authors : Kershaw, N.J.; Burgess, A.W.; Church, N.L.; Luo, C.S.; Adam, T.E.
Deposited on : unknown
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

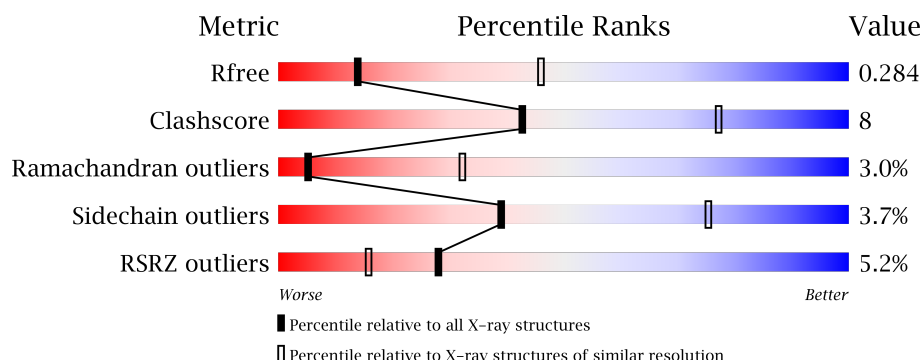
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	531	<div> <div>3%</div> <div>39%</div> <div>8%</div> <div>52%</div> </div>
1	B	531	<div> <div>3%</div> <div>63%</div> <div>10%</div> <div>24%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4996 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.

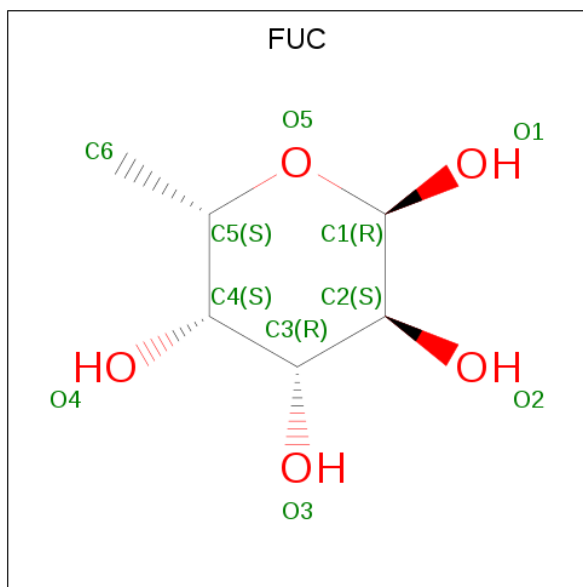
- Molecule 1 is a protein called Delta-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1969	1241	347	357	24			
1	B	401	Total	C	N	O	S	0	0	0
			3017	1862	526	580	49			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	GLN	GLU	conflict	UNP O00548
A	502	GLY	ARG	conflict	UNP O00548
A	510	SER	GLY	conflict	UNP O00548
A	546	GLU	-	expression tag	UNP O00548
A	547	ASN	-	expression tag	UNP O00548
A	548	LEU	-	expression tag	UNP O00548
A	549	TYR	-	expression tag	UNP O00548
A	550	PHE	-	expression tag	UNP O00548
A	551	GLN	-	expression tag	UNP O00548
B	498	GLN	GLU	conflict	UNP O00548
B	502	GLY	ARG	conflict	UNP O00548
B	510	SER	GLY	conflict	UNP O00548
B	546	GLU	-	expression tag	UNP O00548
B	547	ASN	-	expression tag	UNP O00548
B	548	LEU	-	expression tag	UNP O00548
B	549	TYR	-	expression tag	UNP O00548
B	550	PHE	-	expression tag	UNP O00548
B	551	GLN	-	expression tag	UNP O00548

- Molecule 2 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	6	4		

CYS	VAL
PRO	VAL
PRO	ASP
GLY	LEU
THR	THR
THR	GLU
GLY	LYS
ARG	LEU
ASN	GLU
CYS	GLY
SER	GLN
ALA	GLY
PRO	GLY
VAL	PRO
SER	PHE
ARG	PRO
CYS	TRP
GLU	GLU
HIS	ASN
ALA	LEU
PRO	TYR
CYS	PHE
HIS	GLN
ASN	
GLY	
ALA	
THR	
CYS	
HIS	
GLN	
ARG	
GLY	
HIS	
GLY	
TYR	
VAL	
CYS	
GLU	
CYS	
ALA	
ARG	
SER	
TYR	
GLY	
PRO	
ASN	
CYS	
GLN	
PHE	
LEU	
PRO	
GLU	
LEU	
PRO	
PRO	
GLY	
PRO	
ALA	

VAL
VAL
ASP
LEU
THR
GLU
LYS
LEU
GLU
GLY
GLN
GLY
GLY
PRO
VAL
SER
PHE
PRO
TRP
GLU
ASN
LEU
TYR
PHE
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.15Å 118.87Å 134.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.30 – 3.20 89.16 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.30-3.20) 99.8 (89.16-3.20)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.258 , 0.283 0.258 , 0.284	Depositor DCC
R_{free} test set	1998 reflections (6.83%)	DCC
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC

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	0.26	0/2028	0.48	0/2746
1	B	0.26	0/3102	0.48	0/4202
All	All	0.26	0/5130	0.48	0/6948

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Peptide
1	B	142	ARG	Peptide

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	1969	0	1803	34	0
1	B	3017	0	2717	41	0
2	B	10	0	10	0	0
All	All	4996	0	4530	74	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 8.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:O	1:A:143:LEU:HB3	1.38	1.23
1:A:141:GLU:O	1:A:143:LEU:CB	1.89	1.20
1:B:384:SER:HB3	1:B:385:PRO:HD2	1.28	1.16
1:B:384:SER:OG	1:B:385:PRO:HD3	1.52	1.10
1:B:384:SER:CB	1:B:385:PRO:CD	2.34	1.06
1:A:141:GLU:O	1:A:142:ARG:C	2.15	0.84
1:A:141:GLU:O	1:A:143:LEU:HB2	1.80	0.80
1:B:384:SER:HB3	1:B:385:PRO:CD	1.98	0.79
1:B:384:SER:CB	1:B:385:PRO:HD3	2.10	0.76
1:B:302:ALA:HB1	1:B:315:SER:O	1.87	0.75
1:A:151:ARG:NH1	1:A:162:ASP:OD2	2.28	0.65
1:B:384:SER:OG	1:B:385:PRO:CD	2.30	0.65
1:B:57:ARG:NH1	1:B:130:ASP:O	2.31	0.64
1:B:195:ARG:NH2	1:B:197:ASP:OD2	2.30	0.64
1:A:43:ASN:HB3	1:A:142:ARG:O	2.00	0.61
1:B:33:VAL:HB	1:B:170:ASP:HB2	1.81	0.61
1:B:307:THR:HG1	1:B:311:SER:HG	1.46	0.61
1:B:166:SER:HG	1:B:169:THR:HG1	1.48	0.60
1:A:33:VAL:HB	1:A:170:ASP:HB3	1.83	0.59
1:A:31:GLU:O	1:A:172:LYS:N	2.35	0.58
1:A:141:GLU:O	1:A:143:LEU:N	2.37	0.57
1:A:128:HIS:O	1:A:142:ARG:HB2	2.06	0.56
1:B:31:GLU:O	1:B:172:LYS:N	2.38	0.56
1:A:119:THR:HG1	1:B:119:THR:HG1	1.51	0.55
1:A:141:GLU:O	1:A:143:LEU:CA	2.54	0.54
1:B:418:ALA:HB2	1:B:431:CYS:HB3	1.90	0.53
1:A:239:LYS:NZ	1:A:242:GLU:OE1	2.41	0.53
1:B:385:PRO:O	1:B:386:ASP:C	2.46	0.53
1:A:162:ASP:OD1	1:A:163:LEU:N	2.42	0.52
1:B:143:LEU:O	1:B:144:ILE:HG13	2.10	0.52
1:A:36:LYS:NZ	1:A:56:CYS:SG	2.81	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HG	1:A:143:LEU:HD12	1.92	0.52
1:B:166:SER:OG	1:B:169:THR:OG1	2.23	0.51
1:B:384:SER:HG	1:B:385:PRO:HD3	1.71	0.51
1:B:44:CYS:O	1:B:54:CYS:HB3	2.10	0.51
1:B:140:PRO:HG2	1:B:142:ARG:HH12	1.76	0.51
1:B:59:PHE:CE1	1:B:129:THR:HG23	2.46	0.51
1:A:61:ARG:NH2	1:A:75:PRO:HB3	2.25	0.51
1:B:385:PRO:O	1:B:386:ASP:O	2.30	0.50
1:B:65:LYS:HG3	1:B:121:SER:HB2	1.94	0.49
1:B:61:ARG:HH21	1:B:75:PRO:HB3	1.77	0.49
1:B:59:PHE:CE1	1:B:127:LEU:HB2	2.47	0.49
1:A:33:VAL:HA	1:A:91:SER:HB2	1.95	0.48
1:A:65:LYS:HG2	1:A:77:CYS:HA	1.95	0.48
1:B:26:GLU:OE1	1:B:109:ARG:NH1	2.46	0.48
1:B:355:PRO:HB2	1:B:358:PHE:HD1	1.79	0.48
1:B:403:GLU:HG2	1:B:404:LYS:HG3	1.96	0.48
1:B:147:LEU:HB2	1:B:164:HIS:CD2	2.49	0.47
1:A:28:LYS:HB3	1:A:107:PRO:HB3	1.95	0.47
1:A:143:LEU:O	1:A:144:ILE:HG13	2.14	0.47
1:B:36:LYS:HB2	1:B:41:ASN:ND2	2.30	0.47
1:B:127:LEU:HA	1:B:143:LEU:HA	1.97	0.47
1:A:127:LEU:HA	1:A:143:LEU:HA	1.97	0.46
1:B:44:CYS:HA	1:B:128:HIS:CD2	2.50	0.46
1:B:61:ARG:NH2	1:B:75:PRO:HB3	2.30	0.46
1:B:41:ASN:HB3	1:B:44:CYS:SG	2.55	0.46
1:A:124:ILE:HD13	1:A:171:LEU:HD21	1.98	0.45
1:A:124:ILE:HG23	1:A:147:LEU:HB3	1.96	0.45
1:A:140:PRO:HB2	1:A:141:GLU:H	1.62	0.45
1:A:143:LEU:HG	1:A:144:ILE:N	2.32	0.45
1:A:33:VAL:HA	1:A:91:SER:CB	2.47	0.44
1:B:130:ASP:HB3	1:B:132:PRO:HD2	2.00	0.44
1:B:329:ILE:HG22	1:B:348:ASN:H	1.83	0.44
1:A:42:ARG:HG2	1:A:42:ARG:H	1.62	0.42
1:A:131:SER:CB	1:A:132:PRO:HD2	2.50	0.42
1:A:151:ARG:HD3	1:A:151:ARG:HA	1.84	0.42
1:A:73:PRO:HA	1:A:123:ILE:HD13	2.02	0.42
1:B:25:PHE:CD1	1:B:64:LEU:HD11	2.55	0.42
1:A:61:ARG:NH1	1:A:125:GLU:OE1	2.52	0.41
1:A:26:GLU:OE2	1:A:109:ARG:NH1	2.44	0.41
1:B:193:ARG:HA	1:B:194:PRO:HD3	1.93	0.41
1:A:59:PHE:CE1	1:A:127:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ARG:O	1:B:143:LEU:O	2.39	0.40
1:B:106:ASN:HA	1:B:107:PRO:HD2	1.94	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	243/531 (46%)	213 (88%)	21 (9%)	9 (4%)	4	26
1	B	393/531 (74%)	355 (90%)	28 (7%)	10 (2%)	6	38
All	All	636/1062 (60%)	568 (89%)	49 (8%)	19 (3%)	5	32

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	142	ARG
1	B	31	GLU
1	B	33	VAL
1	B	143	LEU
1	B	386	ASP
1	B	425	ASP
1	B	144	ILE
1	B	329	ILE
1	B	440	CYS
1	A	33	VAL
1	A	136	ALA
1	A	143	LEU
1	A	241	GLY
1	B	75	PRO
1	A	75	PRO

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Mol	Chain	Res	Type
1	A	167	GLY
1	B	41	ASN
1	A	144	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	212/440 (48%)	206 (97%)	6 (3%)	49	81
1	B	332/440 (76%)	318 (96%)	14 (4%)	34	72
All	All	544/880 (62%)	524 (96%)	20 (4%)	39	75

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	CYS
1	A	54	CYS
1	A	63	CYS
1	A	142	ARG
1	A	197	ASP
1	A	199	PHE
1	B	30	GLN
1	B	45	CYS
1	B	46	ARG
1	B	56	CYS
1	B	130	ASP
1	B	226	CYS
1	B	294	HIS
1	B	303	THR
1	B	315	SER
1	B	332	CYS
1	B	383	ASP
1	B	384	SER
1	B	431	CYS
1	B	442	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FUC	B	1500	1	9,10,11	0.52	0	13,14,16	1.24	2 (15%)

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
2	FUC	B	1500	1	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1500	FUC	O5-C1-C2	-2.15	107.42	110.79
2	B	1500	FUC	C1-O5-C5	-2.06	107.83	112.39

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

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	253/531 (47%)	0.73	16 (6%)	21 12	42, 84, 134, 158	0
1	B	401/531 (75%)	0.62	18 (4%)	34 21	47, 80, 143, 167	0
All	All	654/1062 (61%)	0.66	34 (5%)	28 16	42, 82, 141, 167	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ASP	3.9
1	A	283	LEU	3.3
1	B	326	GLU	3.2
1	B	370	CYS	2.9
1	B	327	LEU	2.9
1	B	323	ALA	2.9
1	B	356	PRO	2.9
1	B	52	PRO	2.8
1	B	32	PHE	2.7
1	A	186	GLU	2.7
1	A	123	ILE	2.7
1	B	387	GLY	2.6
1	A	122	LEU	2.6
1	A	22	SER	2.5
1	B	22	SER	2.4
1	B	143	LEU	2.4
1	A	264	LEU	2.4
1	A	147	LEU	2.4
1	B	361	LYS	2.3
1	B	39	LEU	2.3
1	B	33	VAL	2.2
1	A	278	GLU	2.2
1	A	90	ASP	2.2
1	B	38	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	424	GLY	2.1
1	B	421	VAL	2.1
1	A	78	THR	2.1
1	B	331	GLU	2.1
1	A	33	VAL	2.1
1	A	124	ILE	2.1
1	B	359	TYR	2.0
1	A	29	LEU	2.0
1	A	240	PRO	2.0
1	A	31	GLU	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	FUC	B	1500	10/11	0.80	0.20	-	142,162,174,177	0

6.5 Other polymers [i](#)

There are no such residues in this entry.