



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5MR2 / pdb_00005mr2
Title : Crystal structure of red abalone VERL repeat 2 with linker at 2.5 Å resolution
Authors : Sadat Al-Hosseini, H.; Raj, I.; Nishimura, K.; De Sanctis, D.; Jovine, L.
Deposited on : 2016-12-21
Resolution : 2.50 Å(reported)

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

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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

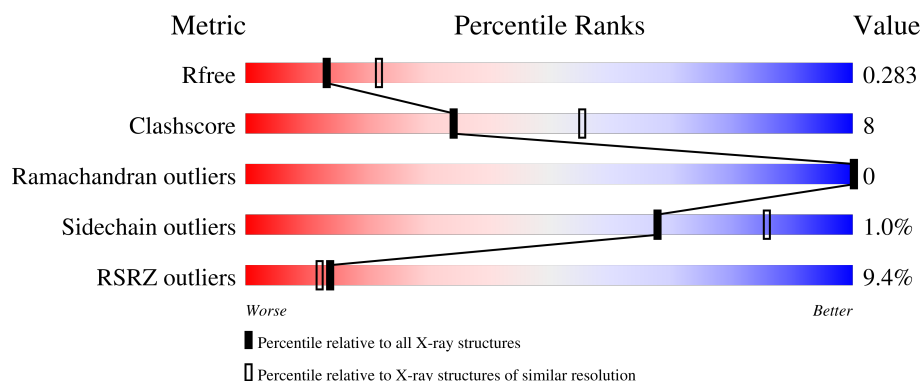
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	134	9% 66% 14% 20%
1	B	134	7% 68% 10% • 21%
1	C	134	6% 64% 13% • 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5056 atoms, of which 2484 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 Vitelline envelope sperm lysin receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	107	Total	C	H	N	O	S	0	0	0
			1663	541	821	136	155	10			
1	B	106	Total	C	H	N	O	S	0	0	0
			1645	536	809	136	155	9			
1	C	105	Total	C	H	N	O	S	0	0	0
			1642	534	812	136	151	9			

There are 42 discrepancies between the modelled and reference sequences:

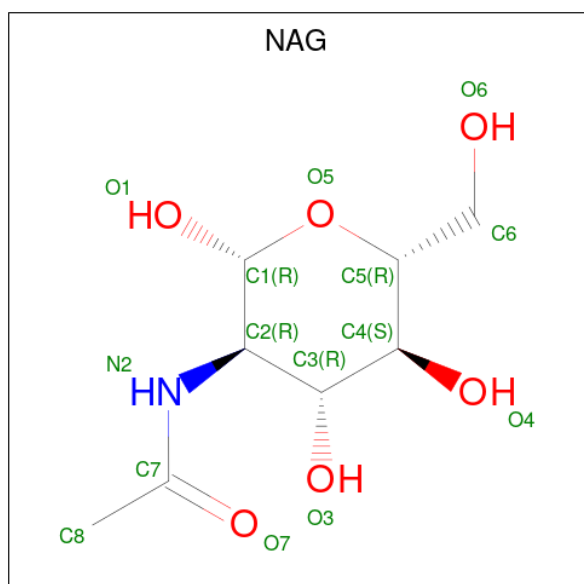
Chain	Residue	Modelled	Actual	Comment	Reference
A	173	GLU	-	expression tag	UNP Q8WR62
A	174	THR	-	expression tag	UNP Q8WR62
A	175	GLY	-	expression tag	UNP Q8WR62
A	293	ALA	SER	engineered mutation	UNP Q8WR62
A	296	ALA	SER	engineered mutation	UNP Q8WR62
A	297	ALA	SER	engineered mutation	UNP Q8WR62
A	299	LEU	-	expression tag	UNP Q8WR62
A	300	GLU	-	expression tag	UNP Q8WR62
A	301	HIS	-	expression tag	UNP Q8WR62
A	302	HIS	-	expression tag	UNP Q8WR62
A	303	HIS	-	expression tag	UNP Q8WR62
A	304	HIS	-	expression tag	UNP Q8WR62
A	305	HIS	-	expression tag	UNP Q8WR62
A	306	HIS	-	expression tag	UNP Q8WR62
B	173	GLU	-	expression tag	UNP Q8WR62
B	174	THR	-	expression tag	UNP Q8WR62
B	175	GLY	-	expression tag	UNP Q8WR62
B	293	ALA	SER	engineered mutation	UNP Q8WR62
B	296	ALA	SER	engineered mutation	UNP Q8WR62
B	297	ALA	SER	engineered mutation	UNP Q8WR62
B	299	LEU	-	expression tag	UNP Q8WR62
B	300	GLU	-	expression tag	UNP Q8WR62
B	301	HIS	-	expression tag	UNP Q8WR62

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP Q8WR62
B	303	HIS	-	expression tag	UNP Q8WR62
B	304	HIS	-	expression tag	UNP Q8WR62
B	305	HIS	-	expression tag	UNP Q8WR62
B	306	HIS	-	expression tag	UNP Q8WR62
C	173	GLU	-	expression tag	UNP Q8WR62
C	174	THR	-	expression tag	UNP Q8WR62
C	175	GLY	-	expression tag	UNP Q8WR62
C	293	ALA	SER	engineered mutation	UNP Q8WR62
C	296	ALA	SER	engineered mutation	UNP Q8WR62
C	297	ALA	SER	engineered mutation	UNP Q8WR62
C	299	LEU	-	expression tag	UNP Q8WR62
C	300	GLU	-	expression tag	UNP Q8WR62
C	301	HIS	-	expression tag	UNP Q8WR62
C	302	HIS	-	expression tag	UNP Q8WR62
C	303	HIS	-	expression tag	UNP Q8WR62
C	304	HIS	-	expression tag	UNP Q8WR62
C	305	HIS	-	expression tag	UNP Q8WR62
C	306	HIS	-	expression tag	UNP Q8WR62

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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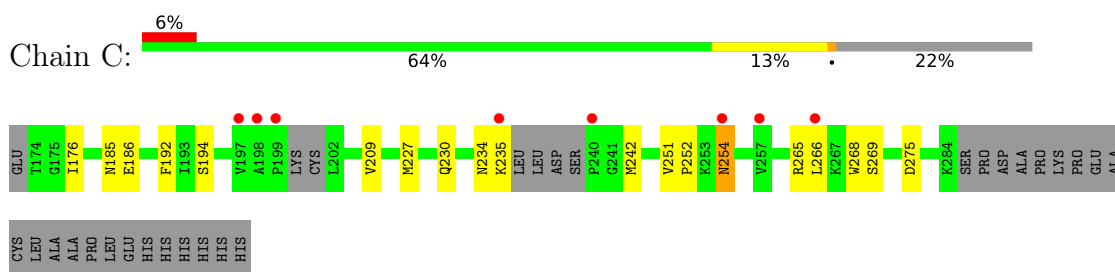
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	6	Total	O	0	0
			6	6		
3	C	13	Total	O	0	0
			13	13		

- Molecule 1: Vitelline envelope sperm lysin receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.92Å 79.19Å 81.24Å 90.00° 102.62° 90.00°	Depositor
Resolution (Å)	47.01 – 2.50 47.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.01-2.50) 99.9 (47.01-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.234 , 0.280 0.238 , 0.283	Depositor DCC
R_{free} test set	1504 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5056	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% 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: NAG

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	0.35	0/863	0.55	0/1174
1	B	0.37	0/858	0.56	0/1168
1	C	0.39	0/852	0.58	0/1158
All	All	0.37	0/2573	0.57	0/3500

There are no bond length outliers.

There are no bond angle outliers.

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	842	821	821	12	0
1	B	836	809	809	14	1
1	C	830	812	812	11	1
2	A	14	14	13	2	0
2	B	14	14	13	0	0
2	C	14	14	13	0	0
3	A	3	0	0	1	0
3	B	6	0	0	1	0
3	C	13	0	0	0	0
All	All	2572	2484	2481	38	1

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 (38) 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:233:ARG:O	1:A:236:LEU:N	2.15	0.79
2:A:900:NAG:O7	2:A:900:NAG:O3	2.04	0.74
1:B:230:GLN:OE1	1:B:242:MET:HE3	1.94	0.67
1:A:254:ASN:OD1	1:A:256:THR:N	2.27	0.65
1:C:254:ASN:OD1	1:C:254:ASN:N	2.29	0.64
1:B:209:VAL:HG21	1:B:227:MET:HE1	1.81	0.63
1:C:209:VAL:HG21	1:C:227:MET:HE1	1.83	0.61
1:C:192:PHE:HD2	1:C:227:MET:HE2	1.67	0.59
1:B:239:SER:HA	1:B:242:MET:SD	2.43	0.59
1:B:254:ASN:OD1	1:B:256:THR:N	2.33	0.58
1:A:279:GLN:OE1	1:B:279:GLN:NE2	2.35	0.56
1:A:209:VAL:HG21	1:A:227:MET:HE1	1.87	0.56
1:A:254:ASN:OD1	1:A:254:ASN:C	2.49	0.54
1:A:192:PHE:HD2	1:A:227:MET:HE2	1.73	0.54
1:B:191:LYS:NZ	3:B:1001:HOH:O	2.38	0.54
1:B:254:ASN:OD1	1:B:254:ASN:C	2.52	0.53
1:B:239:SER:N	1:B:240:PRO:CD	2.73	0.51
1:C:234:ASN:O	1:C:235:LYS:CB	2.59	0.50
1:A:283:PRO:O	1:A:284:LYS:HB2	2.13	0.49
1:A:202:LEU:CD1	1:A:268:TRP:CE3	2.96	0.48
1:C:185:ASN:OD1	1:C:186:GLU:N	2.47	0.48
1:B:192:PHE:HD2	1:B:227:MET:HE2	1.78	0.47
2:A:900:NAG:HO3	2:A:900:NAG:C7	2.12	0.47
1:B:207:MET:HB2	1:B:266:LEU:HD13	1.96	0.47
1:B:204:VAL:HG13	1:B:266:LEU:HD11	1.97	0.46
1:C:230:GLN:OE1	1:C:242:MET:HE3	2.14	0.46
1:C:266:LEU:HD11	1:C:268:TRP:CZ2	2.51	0.45
1:B:204:VAL:CG1	1:B:266:LEU:HD11	2.48	0.44
1:A:177:ASP:O	1:A:194:SER:HA	2.18	0.44
1:C:251:VAL:HG13	1:C:252:PRO:HD2	1.99	0.44
1:A:265:ARG:NH1	1:A:275:ASP:OD1	2.51	0.43
1:B:230:GLN:OE1	1:B:242:MET:CE	2.63	0.43
1:B:192:PHE:HD2	1:B:227:MET:CE	2.30	0.43
1:A:233:ARG:NH2	3:A:1001:HOH:O	2.31	0.42
1:C:192:PHE:HD2	1:C:227:MET:CE	2.30	0.42
1:A:178:TRP:HA	1:A:193:ILE:O	2.21	0.41
1:C:176:ILE:HD11	1:C:194:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ARG:NH1	1:C:275:ASP:OD1	2.54	0.40

All (1) 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:B:267:LYS:HZ1	1:C:269:SER:O[2_655]	1.48	0.12

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	101/134 (75%)	99 (98%)	2 (2%)	0	100	100
1	B	100/134 (75%)	98 (98%)	2 (2%)	0	100	100
1	C	99/134 (74%)	98 (99%)	1 (1%)	0	100	100
All	All	300/402 (75%)	295 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	97/120 (81%)	96 (99%)	1 (1%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	96/120 (80%)	95 (99%)	1 (1%)	68	86
1	C	95/120 (79%)	94 (99%)	1 (1%)	65	84
All	All	288/360 (80%)	285 (99%)	3 (1%)	68	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	B	254	ASN
1	C	254	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	ASN
1	C	222	HIS
1	C	279	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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	$\# Z > 2$
2	NAG	B	900	1	14,14,15	0.56	0	17,19,21	0.65	0
2	NAG	A	900	1	14,14,15	0.72	1 (7%)	17,19,21	0.80	1 (5%)
2	NAG	C	900	1	14,14,15	0.55	0	17,19,21	0.34	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
2	NAG	B	900	1	-	0/6/23/26	0/1/1/1
2	NAG	A	900	1	-	3/6/23/26	0/1/1/1
2	NAG	C	900	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	NAG	C1-C2	2.16	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	NAG	C1-O5-C5	2.60	115.67	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	NAG	O5-C5-C6-O6
2	A	900	NAG	C3-C2-N2-C7
2	A	900	NAG	C4-C5-C6-O6
2	C	900	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	NAG	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

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	107/134 (79%)	0.77	12 (11%) 10 8	54, 77, 126, 175	0
1	B	106/134 (79%)	0.73	10 (9%) 14 12	52, 76, 140, 153	0
1	C	105/134 (78%)	0.66	8 (7%) 20 17	54, 70, 124, 157	0
All	All	318/402 (79%)	0.72	30 (9%) 14 12	52, 74, 135, 175	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	ALA	6.4
1	A	197	VAL	4.4
1	C	199	PRO	4.1
1	A	237	LEU	4.1
1	B	199	PRO	3.7
1	C	257	VAL	3.6
1	A	252	PRO	3.5
1	B	197	VAL	3.4
1	B	184	GLN	3.3
1	C	240	PRO	3.2
1	B	198	ALA	3.2
1	C	198	ALA	3.1
1	A	253	LYS	3.1
1	A	174	THR	3.0
1	B	204	VAL	2.7
1	B	203	ALA	2.7
1	C	254	ASN	2.6
1	B	251	VAL	2.6
1	A	236	LEU	2.6
1	C	235	LYS	2.4
1	A	219	THR	2.4
1	B	202	LEU	2.4
1	A	204	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	197	VAL	2.3
1	B	174	THR	2.3
1	C	266	LEU	2.2
1	A	233	ARG	2.2
1	B	266	LEU	2.0
1	A	268	TRP	2.0
1	A	256	THR	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 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(Å ²)	Q<0.9
2	NAG	A	900	14/15	0.63	0.18	111,133,158,159	0
2	NAG	B	900	14/15	0.63	0.18	127,147,174,177	0
2	NAG	C	900	14/15	0.67	0.16	101,121,147,149	0

6.5 Other polymers [i](#)

There are no such residues in this entry.